

# Temperature Dependence of Physical-Chemical Properties of Selected Chemicals of Environmental Interest. I. Mononuclear and Polynuclear Aromatic Hydrocarbons

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Physical-chemical property data, which control air-water partitioning, namely vapor pressure, aqueous solubility and Henry's law constant over the environmentally relevant temperature range of 5–50 °C, are compiled and reviewed for the mononuclear aromatic and polynuclear aromatic hydrocarbons. Corresponding enthalpies of phase transition are also reported. As result of a critical review, selected values are given at 25 °C, and where possible equations expressing the temperature dependence are given. Twenty-one aromatic hydrocarbons are studied, with approximately 300 references. © 2000 American Institute of Physics. [S0047-2689(90)00101-5]

Key words: aqueous solubility, aromatic hydrocarbons, Henry's law constant, physical-chemical properties, temperature dependence, vapor pressure.

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## 1. Introduction

It has long been recognized that key physical-chemical properties which control the fate of organic chemicals in the environment, especially in air-water systems, are: aqueous solubility, vapor pressure, and Henry's law constant or the air-water partition coefficient. Values of these properties are generally reported in the literature at ambient or standard temperatures of 20 or 25 °C. Environmentally important temperatures, however, vary considerably, thus reliable data are required on the temperature dependence of these properties. For example, the significantly lower air-water partition coefficients at low water temperatures may cause net air to water diffusion with the direction changing in summer when the partition coefficient increases [Hornbuckle *et al.* (1994)]. Recently, Della Site (1997) reviewed and reported vapor pressures of organic chemicals of environmental interest and presented vapor pressure equations. In this paper, we compile and report experimentally determined aqueous solubilities, vapor pressures, and Henry's law constants of mono-

nuclear and polynuclear aromatic hydrocarbons over a range of temperatures. As result of this critical review, we recommend values at 25 °C and, where possible, provide equations for estimating these properties over the temperature range of 5–50 °C.

## 2. Physical-Chemical Properties

The fundamental thermodynamic relationships between solubilities, vapor pressure, and Henry's law constant have been discussed previously by Mackay and Shiu (1981) and Mackay (1991) and only the essential points are summarized here.

The fugacity of a solute in an aqueous solution,  $f$  (Pa), can be defined as

$$f = x \gamma f_R, \quad (1)$$

where  $x$  is mole fraction in solution,  $\gamma$  is the activity coefficient (Raoult's law convention such that  $\gamma$  approaches 1.0 when  $x$  approaches 1.0), and  $f_R$  is the reference fugacity or approximately the vapor pressure of the pure liquid solute.

The organic compounds considered here are sparingly soluble in water, the most soluble being benzene at 1780 g/m<sup>3</sup> or 1.78 g/L. Solutions are thus necessarily dilute with mole fractions less than 0.0005. In such systems activity coefficients are regarded as independent of concentration and are equal to the infinite dilution values.

The fugacity in the vapor (air) phase can be approximated for these solutes as the partial pressure

$$f = y \phi p_T \approx p, \quad (2)$$

where  $y$  is solute mole fraction,  $\phi$  is the fugacity coefficient (which is close to unity in value for nonassociating substances at environmental pressures and temperatures),  $p_T$  is total pressure (Pa), and  $p$  is partial pressure (Pa). It follows that a Henry's law constant (HLC) with units of pressure can be expressed as

$$k_H = p/x = \gamma f_R. \quad (3)$$

More commonly in environmental science, concentration in the aqueous phase is expressed on a volumetric basis, e.g.,  $c$  in mol/m<sup>3</sup> which is also  $x/v$ , where  $v$  is the molar volume of the aqueous solution and is usually about  $18 \times 10^{-6}$  m<sup>3</sup>/mol. The conventional Henry's law constant  $H$ (Pa·m<sup>3</sup>/mol) is thus given by

$$H = p/c_W = v \gamma f_R. \quad (4)$$

The dimensionless air-water partition coefficient  $K_{AW}$  is defined by

$$K_{AW} = c_A / c_W = H/RT, \quad (5)$$

where  $R$  is the gas constant (8.314 Pa·m<sup>3</sup>/mol·K),  $T$  is the absolute temperature (K), and  $c_A$  is the concentration in air (mol/m<sup>3</sup>) which is  $p/RT$ ; while  $C_W$ (mol/m<sup>3</sup>) is the water solubility.

Under saturation conditions  $p$  becomes the vapor pressure and  $c$  the aqueous solubility denoted as  $p^s$  and  $c_W^s$ , and it is















TABLE I. Physical constants and thermodynamic properties of aromatic hydrocarbons—Continued

Compound	MW	mp <i>t</i> /°C	bp <i>t</i> /°C	$\Delta_{fu}H$ kJ·mol <sup>-1</sup>	at <i>t</i> /°C	$\Delta_{vap}H$ kJ·mol <sup>-1</sup>	at <i>t</i> /°C	$\Delta_{sub}H$ kJ·mol <sup>-1</sup>	at <i>t</i> /°C	Reference	
2-Methylanthracene <chem>C15H12</chem> [613-12-7]	192.26	209	359 subl			56.50	bp	97.50	25	Zwolinski & Wilhoit 1971	
Phenanthrene <chem>C14H10</chem> [85-01-8]	178.23	101	339	18.619 18.62 16.443 18.62 18.48	96.30 Tsonopoulos 1970 Osborn & Douslin 1975 de Kruij 1980 Weast 1982-3	Parks & Huffman 1931 Tsonopoulos 1970 Osborn & Douslin 1975 de Kruij 1980 Weast 1982-3	52.97 70.793 55.60	338.5 99.24 bp	99.70 94.8 100.4 100.5 70.39 94.6 91.80 103.34 86.61 92.88 99.24 87.2 90.50 92.50 59.35 95.0 91.80 95.0	119.4 85-119 78.13 25 80-126 10-50 25 40-100 102.6 101.3 100.0 42 0-60 52-90 51.88 25 25 10-50 45 30-60	Malaspina <i>et al.</i> 1973 Macknick & Prausnitz 1979 de Kruij 1980 de Kruij 1980 Weast 1982-83 Bender <i>et al.</i> 1983 Sonnefeld <i>et al.</i> 1983 Dean 1985 Rordorf 1985, 1986, 1987 Hansen & Eckert 1986 Dean 1992 Oja & Suuberg 1998
1-Methylphenanthrene <chem>C15H12</chem> [832-69-6]	192.26	123	359							Mortimer & Murphy 1923	
Fusac <chem>C16H10</chem> [129-00-0]	202.26	156	393	15.31		Wauchope & Gotzen 1972				Inokuchi <i>et al.</i> 1952	
Fluoranthene <chem>C16H10</chem> [206-44-0]	202.26	111	375	49.37 47.70		Casellato <i>et al.</i> 1973 Hinckley <i>et al.</i> 1990				Bradley & Cleasby 1953	
Chrysene <chem>C18H12</chem> [218-01-9]	228.3	255	448							Hoyer & Peperle 1958	
Triphenylene <chem>C18H12</chem> [217-59-4]	228.3	199	438							Malaspina <i>et al.</i> 1973	
Naphthalene <chem>C18H12</chem> [92-24-0]	228.3	357	450 subl							Yamasaki <i>et al.</i> 1982	
Benz[a]anthracene <chem>C18H12</chem> [56-55-3]	228.3	156.9	435 subl	22.30		Haines & Sandler 1995				Yamasaki <i>et al.</i> 1984	
Triphenylmethane <chem>C19H16</chem> [519-73-3]	244.34	93.4	360							Yamasaki <i>et al.</i> 1984	

## PROPERTIES OF ENVIRONMENTAL INTEREST

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TABLE 1. Physical constants and thermodynamic properties of aromatic hydrocarbons—Continued

Compound	MW	mp t/°C	bp t/°C	$\Delta_{\text{fus}}H$ kJ·mol <sup>-1</sup>	at t/°C	Reference	$\Delta_{\text{vap}}H$ kJ·mol <sup>-1</sup>	at t/°C	$\Delta_{\text{sub}}H$ kJ·mol <sup>-1</sup>	at t/°C	Reference
Benzo[ <i>a</i> ]pyrene C <sub>20</sub> H <sub>12</sub> [50-32-8]	252.30	176.4	495	15.10		Haines & Sandler 1995			100.0	25	Dean 1992
Benzo[ <i>e</i> ]pyrene H <sub>20</sub> H <sub>12</sub> [192-97-2]	252.30	178.8	493						118.4	85–158	Murray <i>et al.</i> 1974
Perylene C <sub>20</sub> H <sub>12</sub> [198-55-0]	252.30	277	495	23.51		Tsonopoulos 1970			118.4		Yamasaki <i>et al.</i> 1984
									119.1	86–150	Murray <i>et al.</i> 1974
									119.2		Yamasaki <i>et al.</i> 1984
									126.4	142	Inokuchi <i>et al.</i> 1952
									140.2	110–180	Hoyer & Peperle 1958
									125.52	25	Dean 1985
									132.6	118–151	Oja & Suuberg 1998
Benzo[ <i>b</i> ]fluoranthene C <sub>20</sub> H <sub>12</sub> [205-99-2]	252.32	166	481								
Benzo[ <i>k</i> ]fluoranthene C <sub>20</sub> H <sub>12</sub> [207-08-9]	252.32	198–217	481						130.1	90–157	Murray <i>et al.</i> 1974
9,10-Dimethylbenz[ <i>a</i> ]- anthracene C <sub>20</sub> H <sub>16</sub> [57-97-6]	256.35	123.5		22.09		Kelley & Rice 1964	112.9	106–135	135.4	106–135	Kelley & Rice 1964
3-Methylcholanthrene C <sub>21</sub> H <sub>16</sub> [56-49-5]	268.36	179.5							127.2	128–152	Kelley & Rice 1964
Benzo[ <i>ghi</i> ]perylene C <sub>22</sub> H <sub>12</sub> [191-24-2]	276.34	278									
Pentacene C <sub>22</sub> H <sub>14</sub> [135-48-8]	278.36	>300					154	239.44	de Kruif 1980		
							184	25	de Kruif 1980		
Dibenz[ <i>a, c</i> ]anthracene C <sub>22</sub> H <sub>14</sub> [215-58-7]	278.36	205					156.9	170–200	Oja & Suuberg 1998		
Dibenz[ <i>a, h</i> ]anthracene C <sub>22</sub> H <sub>14</sub> [53-70-3]	278.36	270	524				139.1	166.68	de Kruif 1980		
Coronene C <sub>24</sub> H <sub>12</sub> [191-07-1]	300.36	440					159	25	de Kruif 1980		
							141.6	176.45	de Kruif 1980		
							162.6	25	de Kruif 1980		
							148.5	134	Inokuchi 1951		
							144.3	160–240	Hoyer & Peperle 1958		
							135.9	154–292	Murray <i>et al.</i> 1974		
							133.1	148–231	Oja & Suuberg 1998		

\*Note:  $\Delta_{\text{fus}}H$  - enthalpy of fusion,  $\Delta_{\text{vap}}H$  - enthalpy of vaporization,  $\Delta_{\text{sub}}H$  - enthalpy of sublimation. mp - melting point in °C; bp - boiling point in °C; tp - triple point in °C.

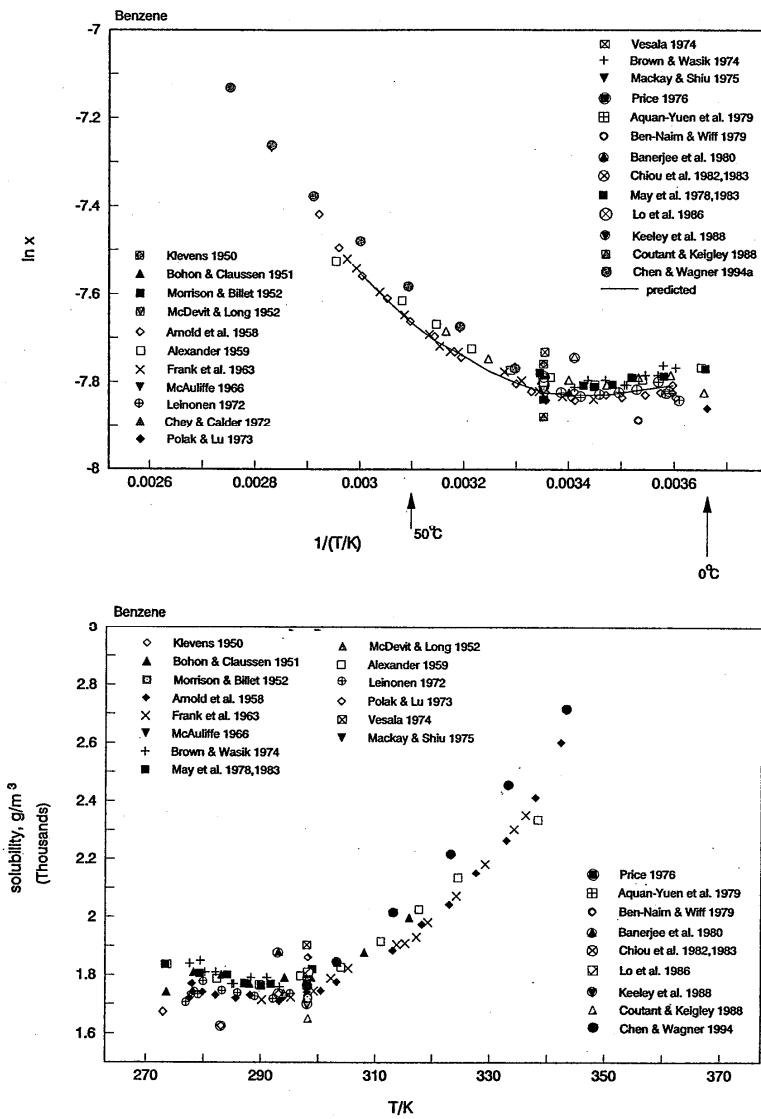


FIG. 1. Logarithm of mole fraction solubility vs  $1/T$  for benzene.

common to estimate  $H$  as  $p_s^s/c_w^s$  from reported vapor pressure and solubility data. This equation applies regardless of whether the solute is solid or liquid, although it should not be applied when there is appreciable miscibility between water and the liquid solute. When the solute is a gas, i.e.,  $p^s$  exceeds  $p_T$ , the solubility is a function of pressure and may be reported at atmospheric pressure or at the higher vapor pressure.

When comparing solubilities or vapor pressures of homologous series it is essential to eliminate the variable effect of crystal structure on the melting point and other solid properties by comparing values of the liquid state. The ratio of solid to liquid properties (the fugacity ratio  $F$ ) is usually estimated from

$$F = c_s^s/c_L^s = p_s^s/p_L^s = \exp[-\Delta_{\text{fus}}S \cdot (T_M/T - 1)/R], \quad (6)$$

where subscripts  $S$  and  $L$  refer to solid and liquid states and  $T_M$  is the melting point (K) and  $\Delta_{\text{fus}}S$  is the entropy of fu-

sion, a value of 56 J/mol·K being a commonly assumed entropy of fusion for intermediate size rigid organic molecules (Yalkowsky, 1979). Since  $p_L^s$  is approximately  $f_R$ , the reference fugacity, it follows that for a liquid solute  $x^s\gamma$  is approximately 1.0 and for solids it is  $p_s^s/p_L^s$ , the fugacity ratio.

In summary for liquids, from a knowledge of  $p_L^s$  and  $c_w^s$  (or  $v$  and  $\gamma$  and  $x^s$ ),  $H$  and  $K_{\text{AW}}$  can be estimated. For solids,  $H$  can be estimated from  $p_s^s$  and  $c_s^s$  or if  $\gamma$  is available from structure property relationships,  $c_s^s$  can be estimated from  $T_M$ ,  $\gamma$  and  $v$ . In practice, since experimental determination of these properties can be difficult, it is preferable to measure solubility, vapor pressure, and Henry's law constant and perform a consistency check.

Other theoretical aspects including a discussion of quantitative structure property relationships (QSPRs) and how these properties influence environmental fate are reviewed in

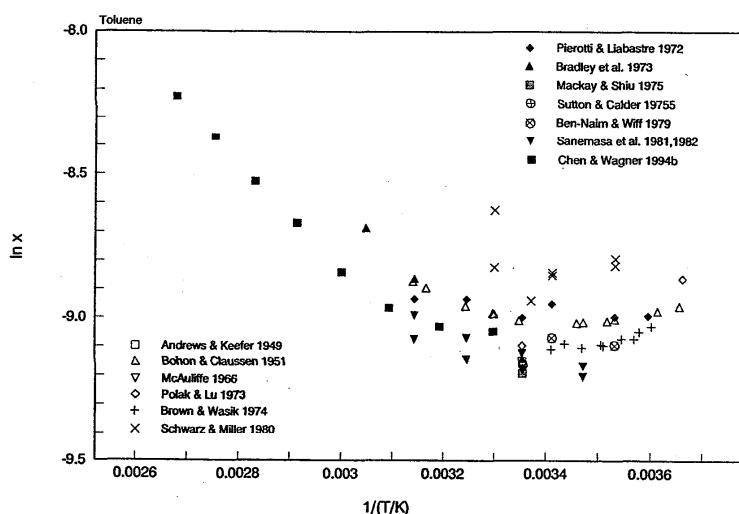


FIG. 2. Logarithm of mole fraction solubility vs  $1/T$  for toluene.

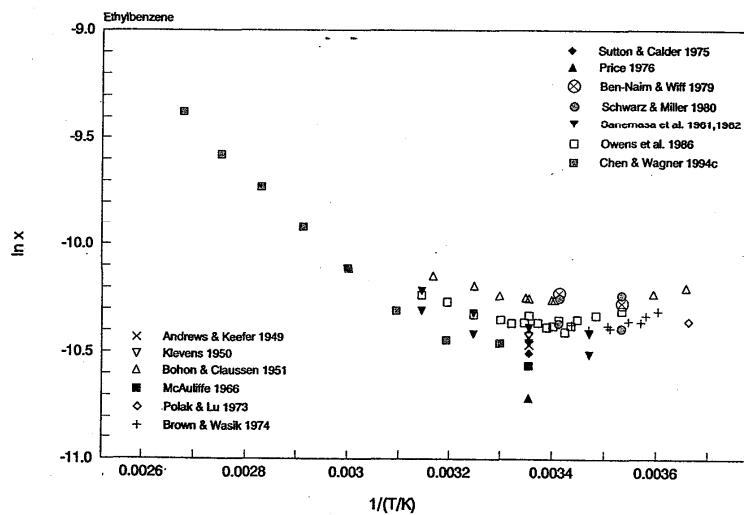


FIG. 3. Logarithm of mole fraction solubility vs  $1/T$  for ethylbenzene.

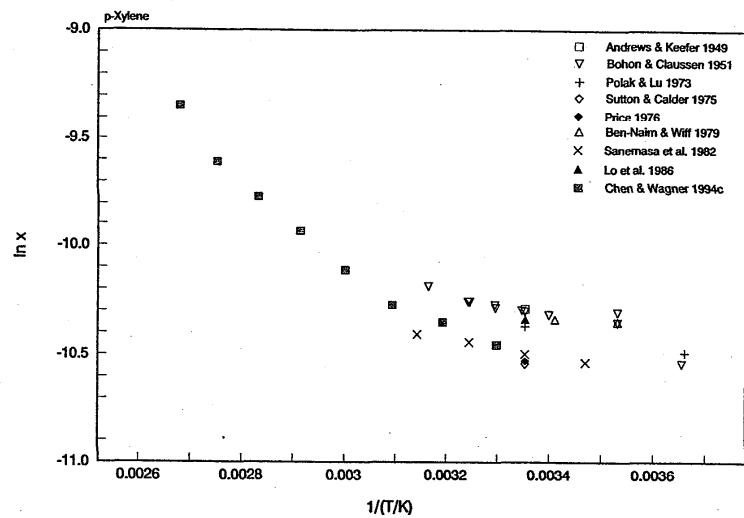


FIG. 4. Logarithm of mole fraction solubility vs  $1/T$  for p-xylene.

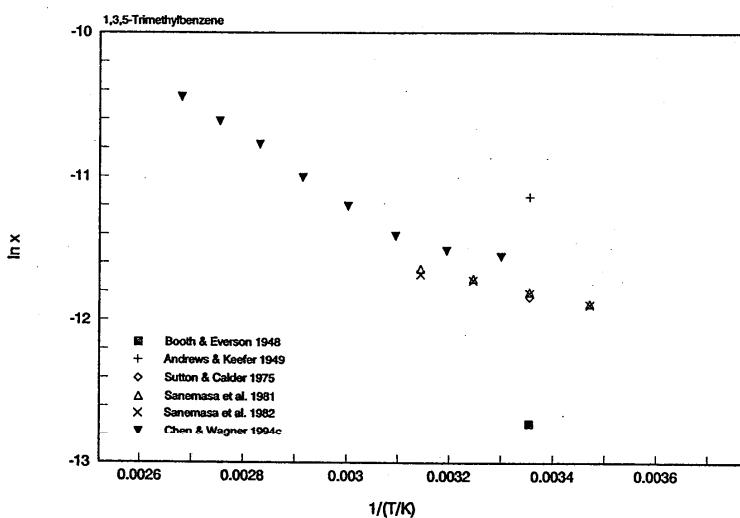


FIG. 5. Logarithm of mole fraction solubility vs  $1/T$  for 1,3,5-trimethylbenzene.

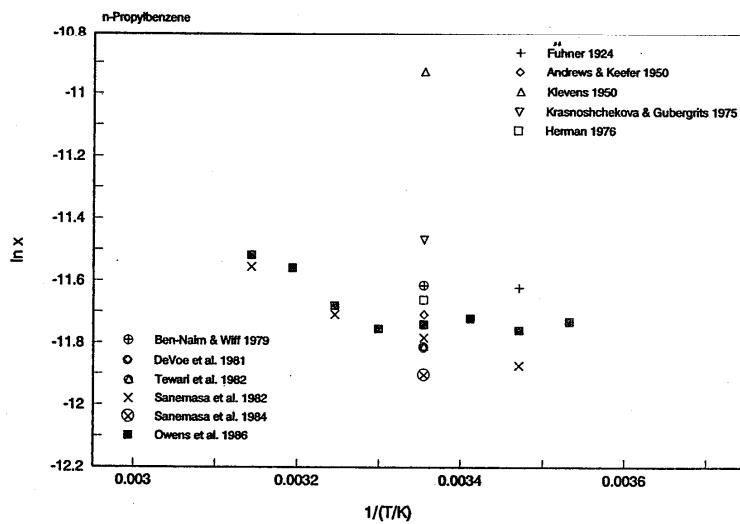


FIG. 6. Logarithm of mole fraction solubility vs  $1/T$  for *n*-propylbenzene.

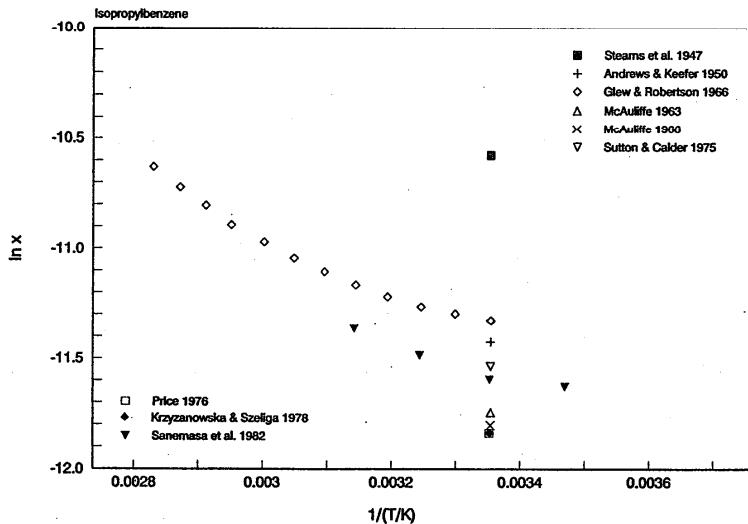


FIG. 7. Logarithm of mole fraction solubility vs  $1/T$  for isopropylbenzene.

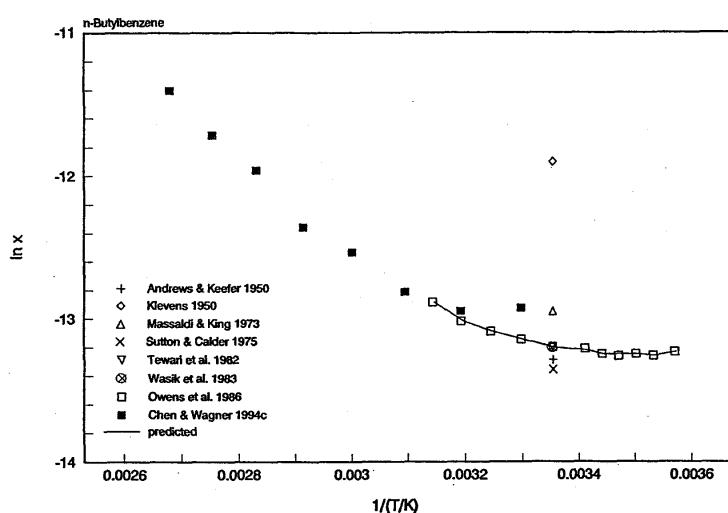


FIG. 8. Logarithm of mole fraction solubility vs  $1/T$  for *n*-butylbenzene.

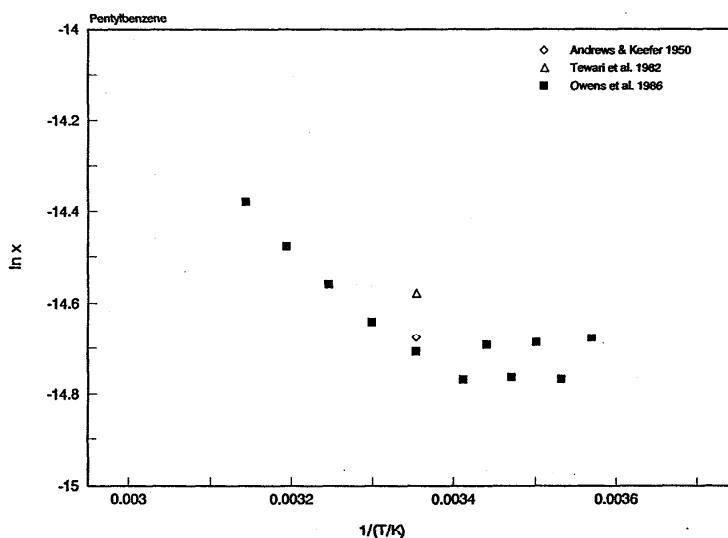


FIG. 9. Logarithm of mole fraction solubility vs  $1/T$  for *n*-pentylbenzene.

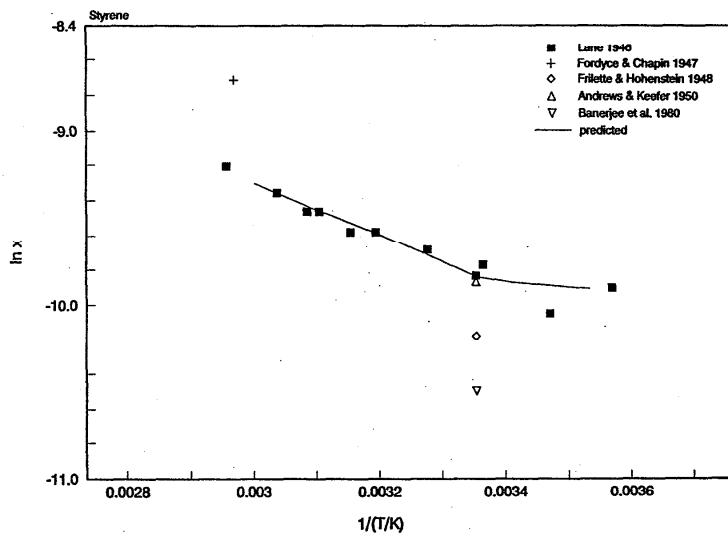


FIG. 10. Logarithm of mole fraction solubility vs  $1/T$  for styrene.

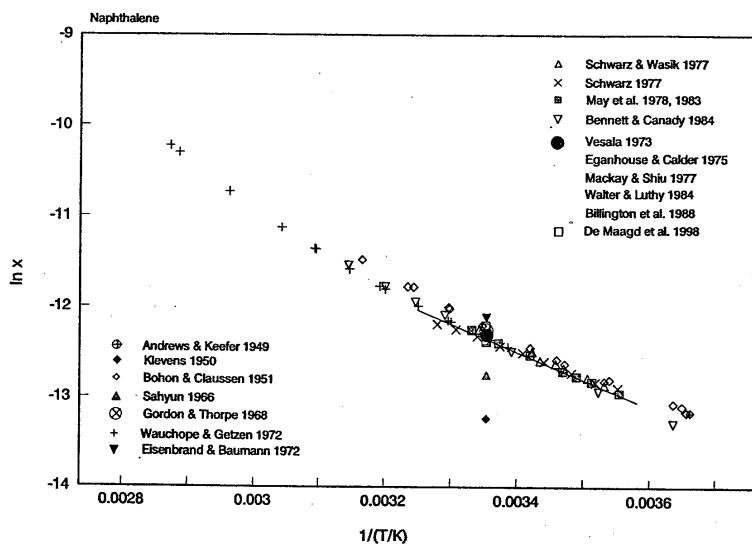


FIG. 11. Logarithm of mole fraction solubility vs  $1/T$  for naphthalene.

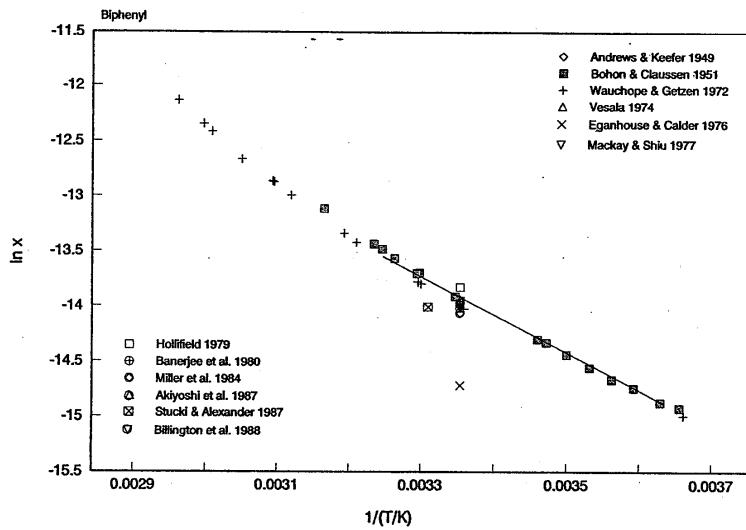


FIG. 12. Logarithm of mole fraction solubility vs  $1/T$  for biphenyl.

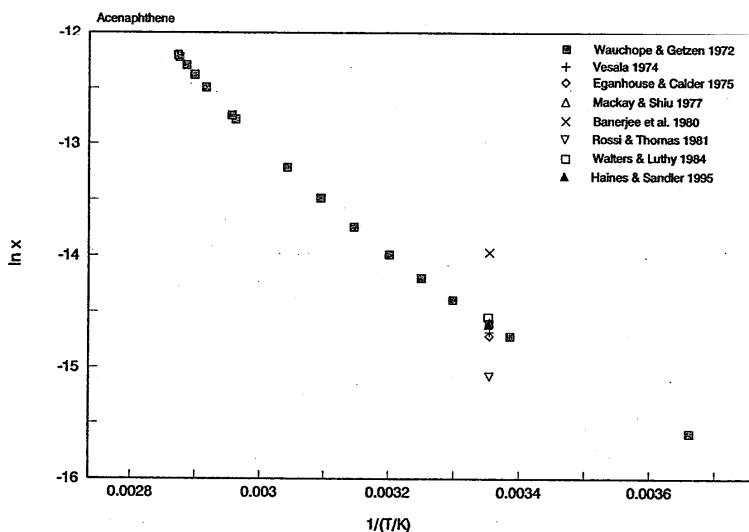


FIG. 13. Logarithm of mole fraction solubility vs  $1/T$  for acenaphthene.

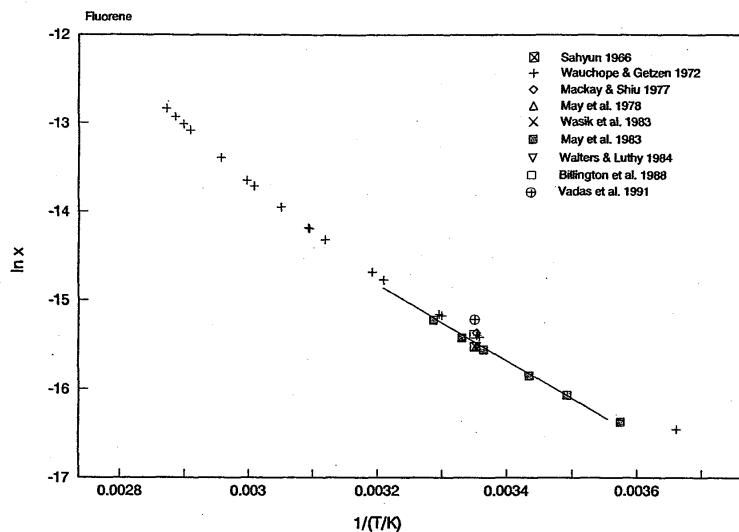


FIG. 14. Logarithm of mole fraction solubility vs  $1/T$  for fluorene.

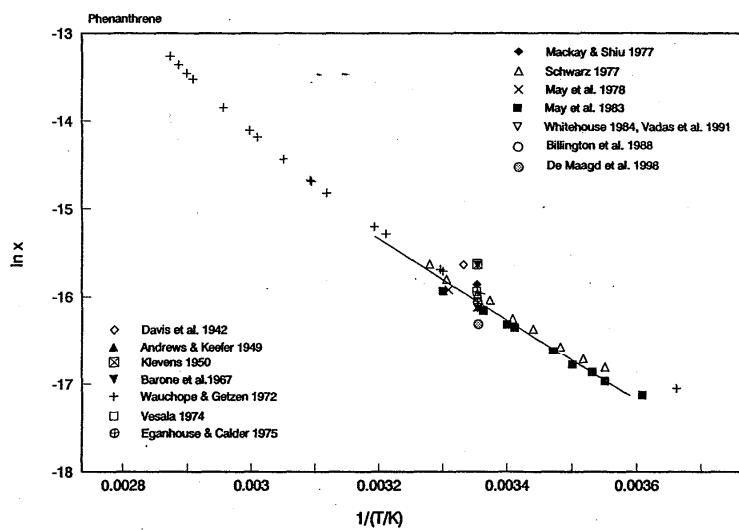


FIG. 15. Logarithm of mole fraction solubility vs  $1/T$  for phenanthrene.

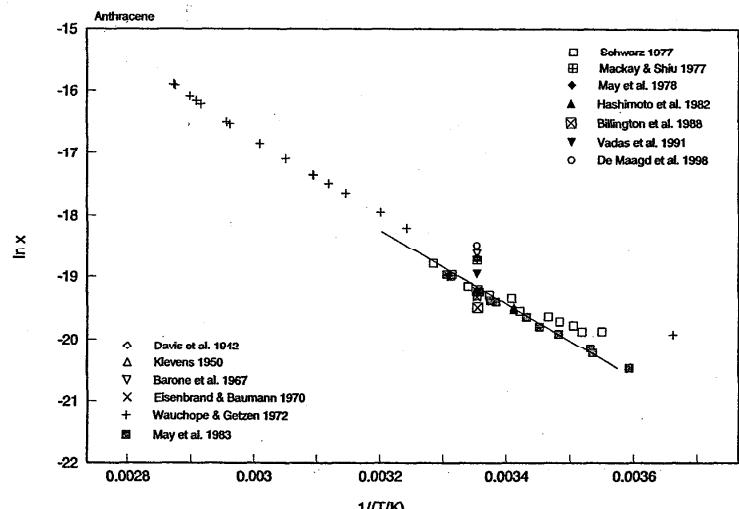


FIG. 16. Logarithm of mole fraction solubility vs  $1/T$  for anthracene.

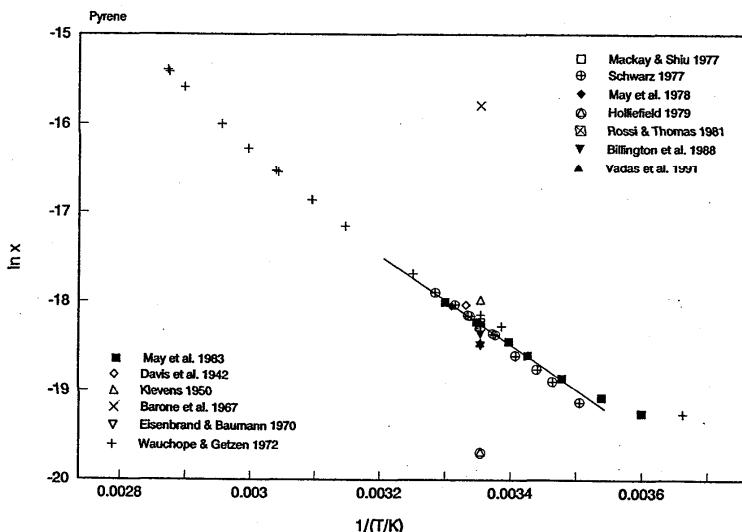


FIG. 17. Logarithm of mole fraction solubility vs  $1/T$  for pyrene.

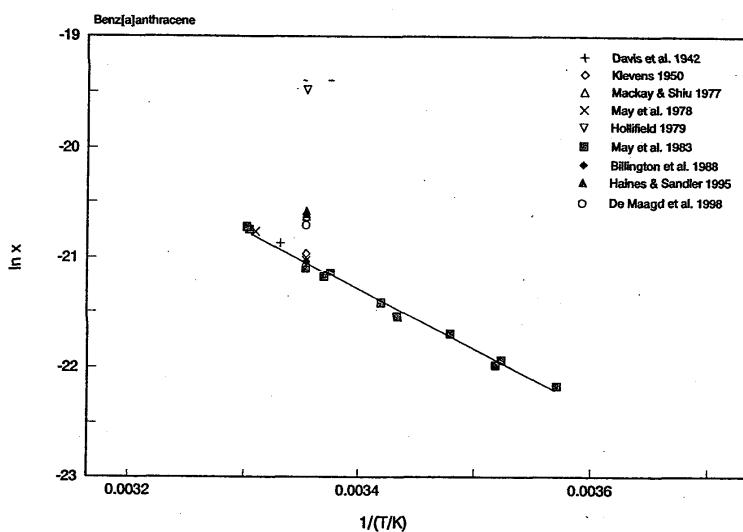


FIG. 18. Logarithm of mole fraction solubility vs  $1/T$  for benzo[a]anthracene.

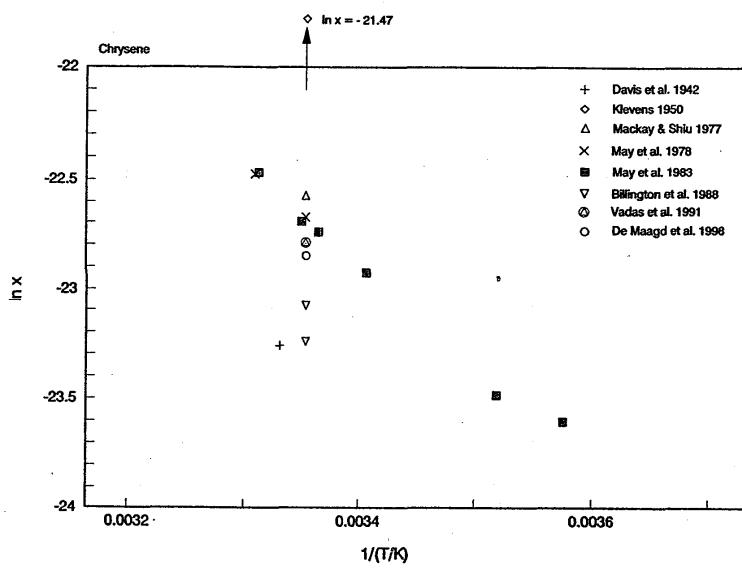


FIG. 19. Logarithm of mole fraction solubility vs  $1/T$  for chrysene.

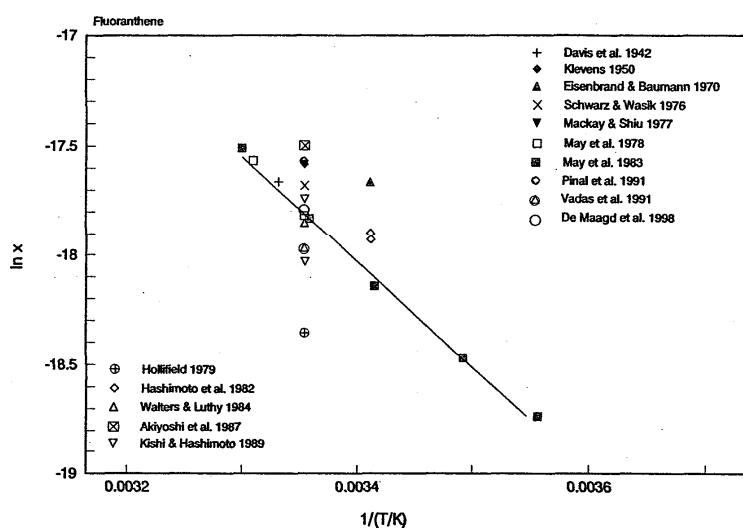


FIG. 20. Logarithm of mole fraction solubility vs  $1/T$  for fluoranthene.

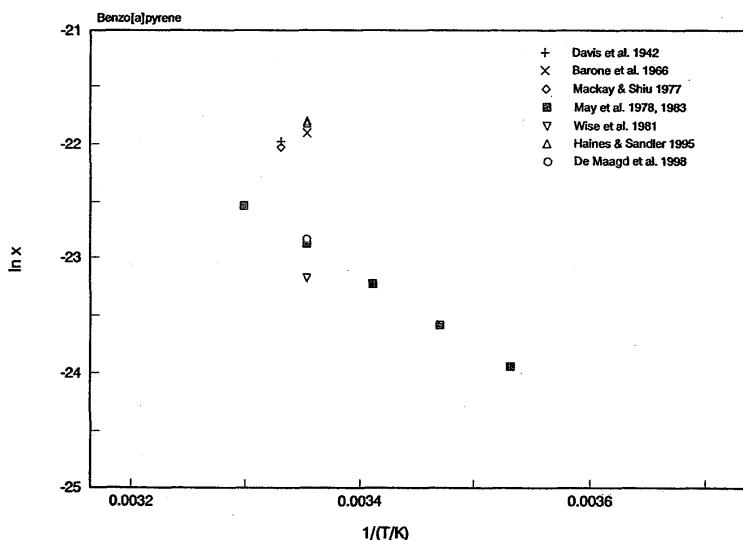


FIG. 21. Logarithm of mole fraction solubility vs  $1/T$  for benzo[*a*]pyrene.

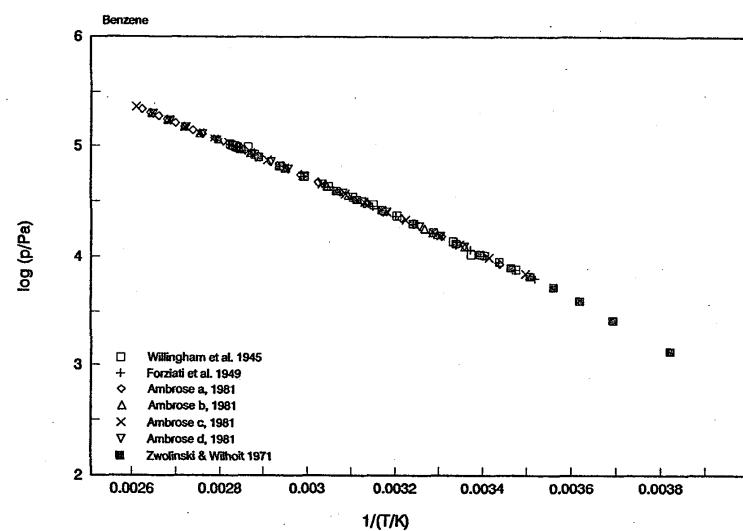


FIG. 22. Logarithm of vapor pressure vs  $1/T$  for benzene.

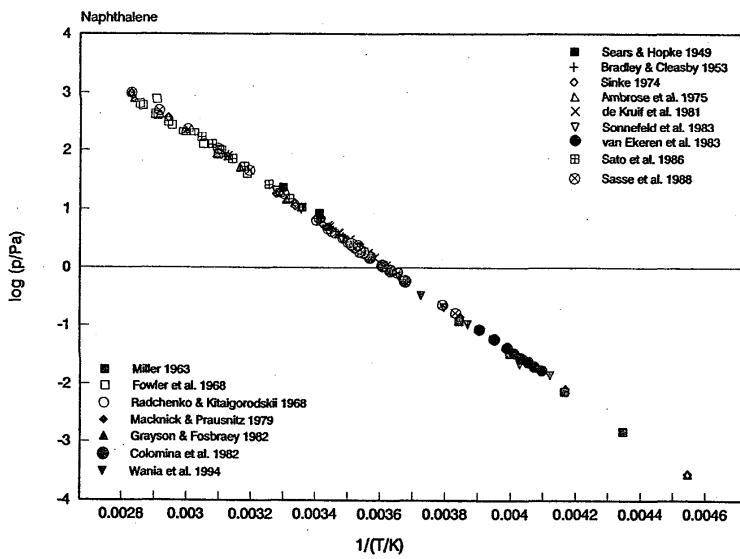


FIG. 23. Logarithm of vapor pressure vs  $1/T$  for naphthalene.

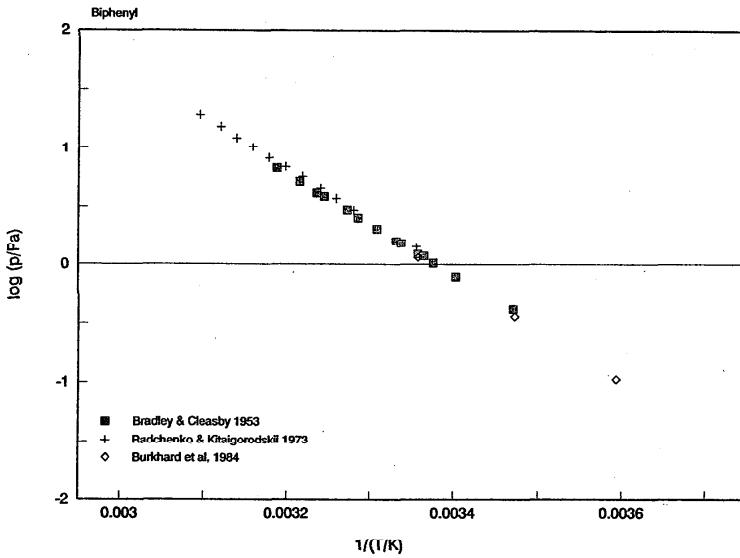


FIG. 24. Logarithm of vapor pressure vs  $1/T$  for biphenyl.

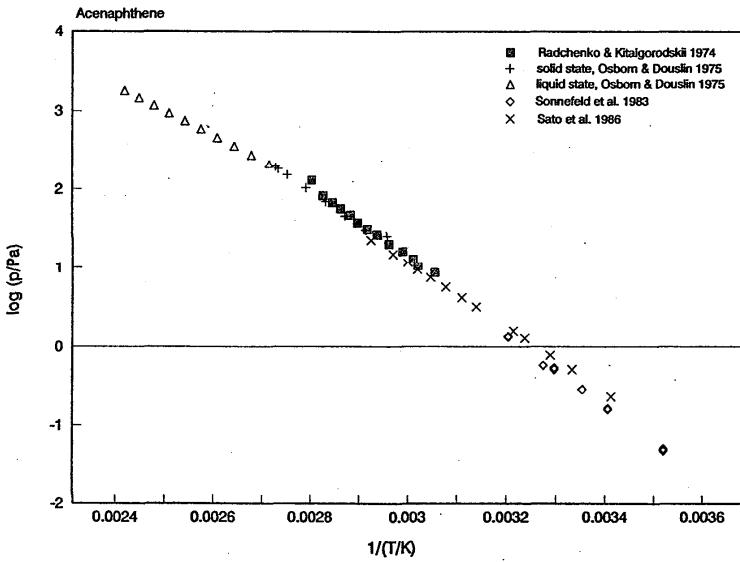


FIG. 25. Logarithm of vapor pressure vs  $1/T$  for acenaphthene.

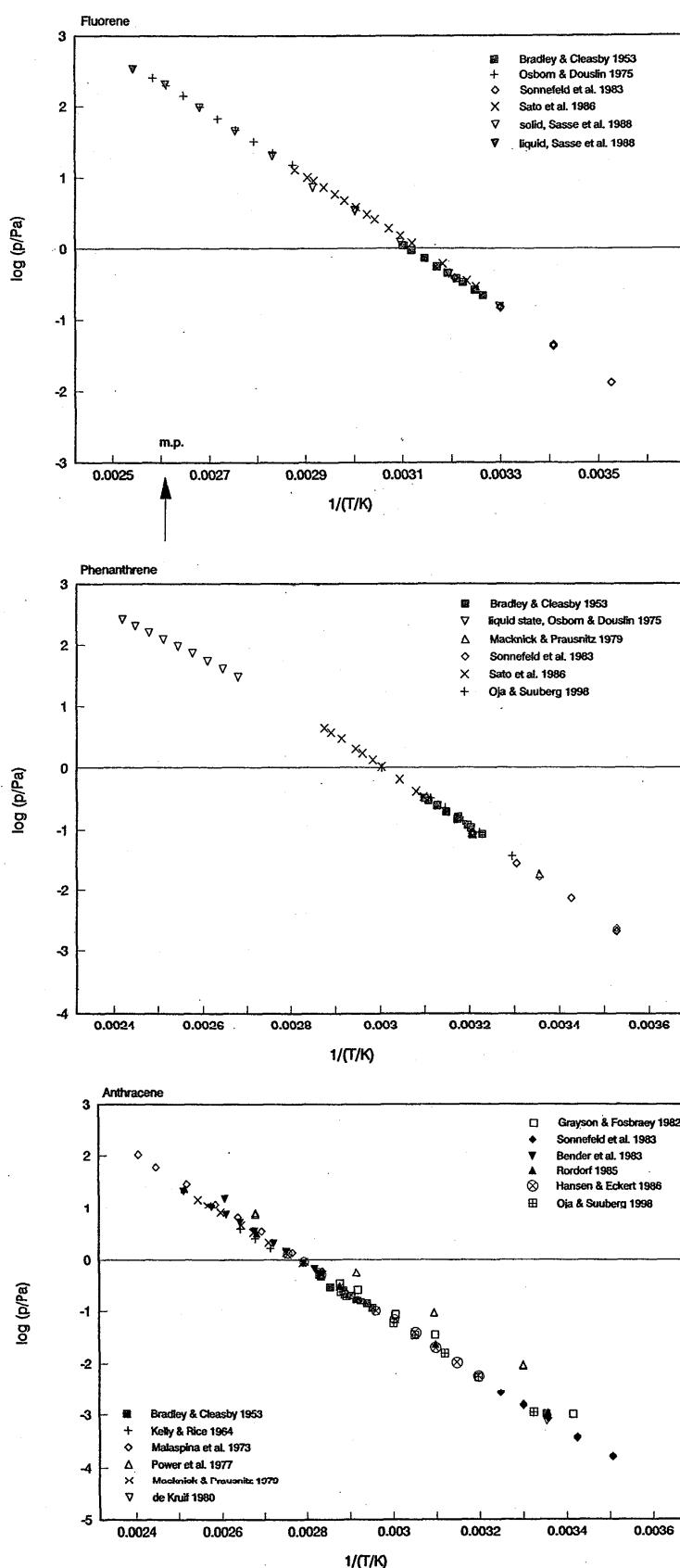
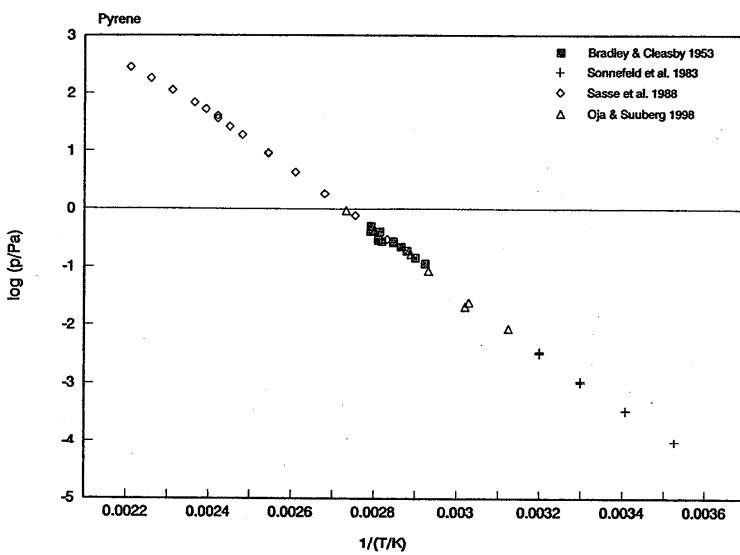
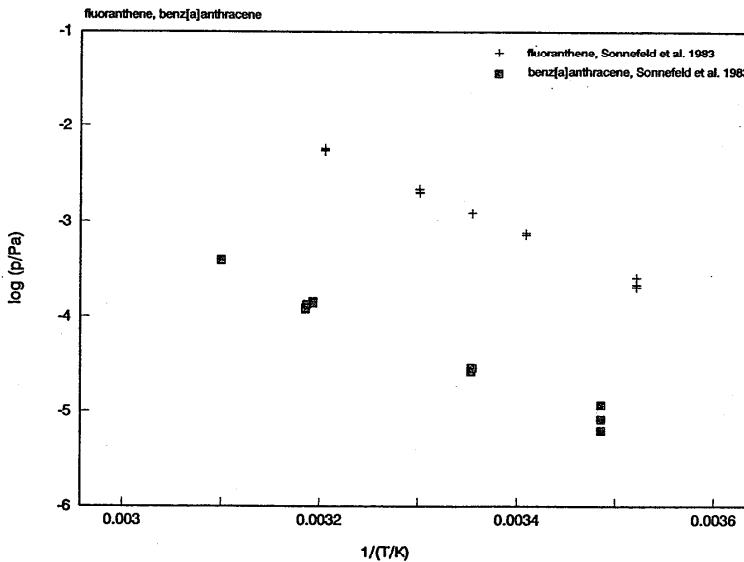
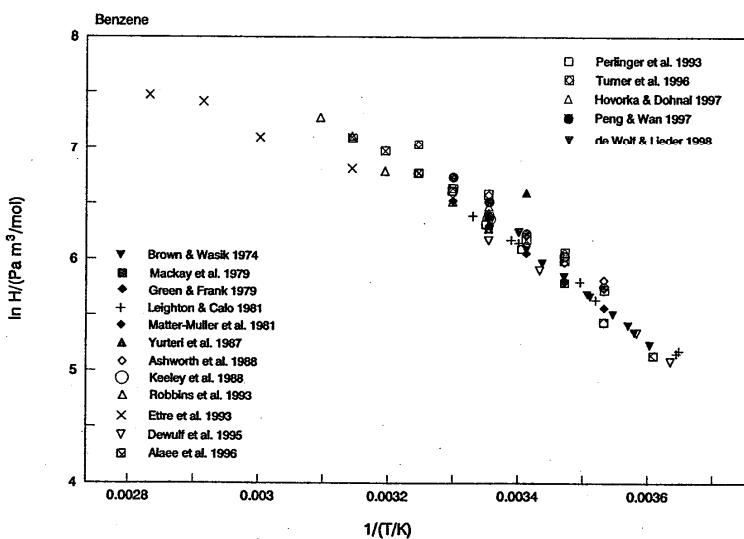


FIG. 26. Logarithm of vapor pressure vs  $1/T$  for fluorene.

FIG. 27. Logarithm of vapor pressure vs  $1/T$  for phenanthrene.

FIG. 28. Logarithm of vapor pressure vs  $1/T$  for anthracene.

FIG. 29. Logarithm of vapor pressure vs  $1/T$  for pyrene.FIG. 30. Logarithm of vapor pressure vs  $1/T$  for fluoranthene, benzo[a]anthracene.FIG. 31. Logarithm of Henry's law constant vs  $1/T$  for benzene.

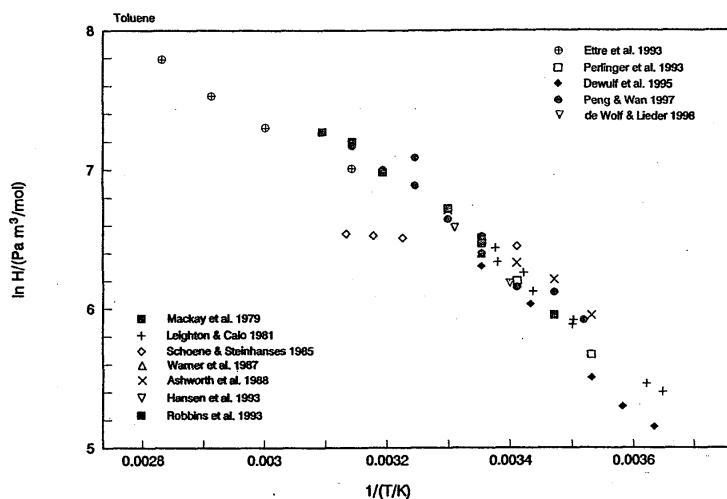


FIG. 32. Logarithm of Henry's law constant vs  $1/T$  for toluene.

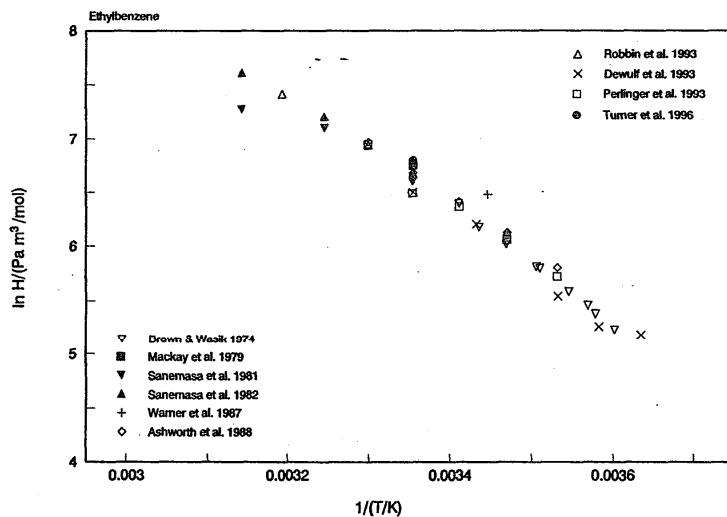


FIG. 33. Logarithm of Henry's law constant vs  $1/T$  for ethylbenzene.

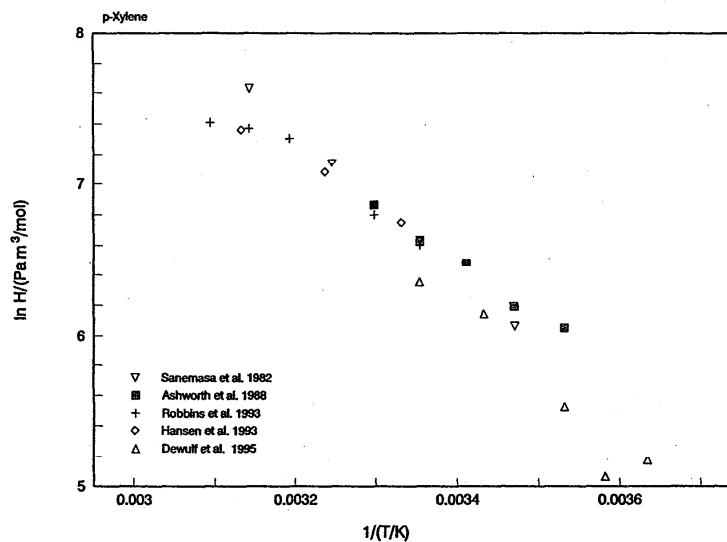


FIG. 34. Logarithm of Henry's law constant vs  $1/T$  for *p*-xylene.

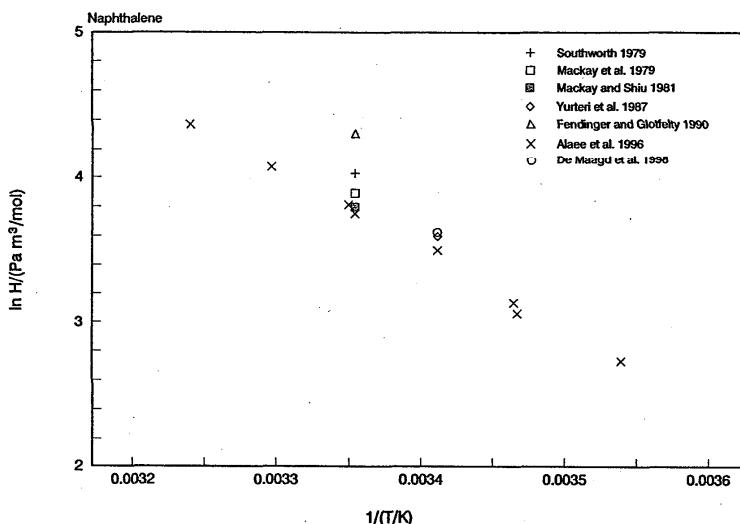


FIG. 35. Logarithm of Henry's law constant vs  $1/T$  for naphthalene.

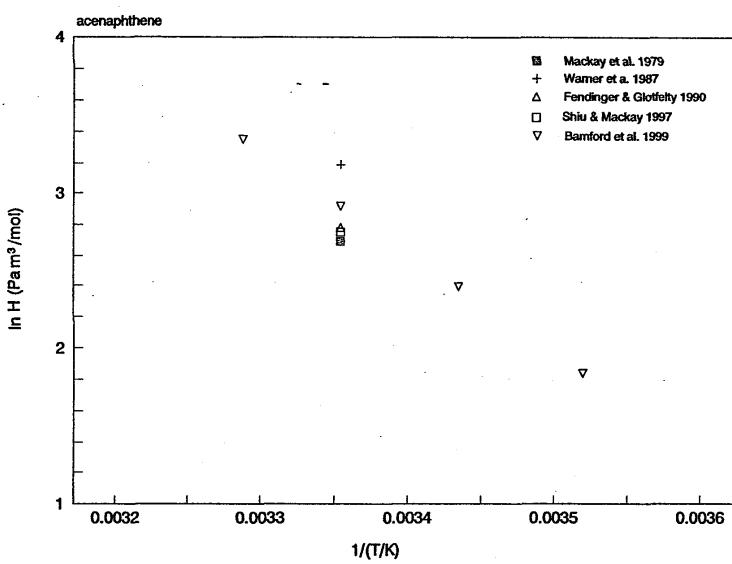


FIG. 36. Logarithm of Henry's law constant vs  $1/T$  for acenaphthene.

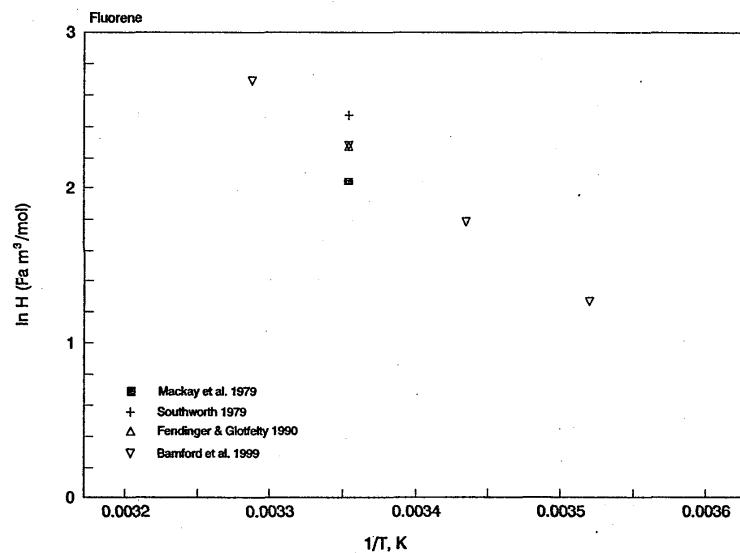


FIG. 37. Logarithm of Henry's law constant vs  $1/T$  for fluorene.

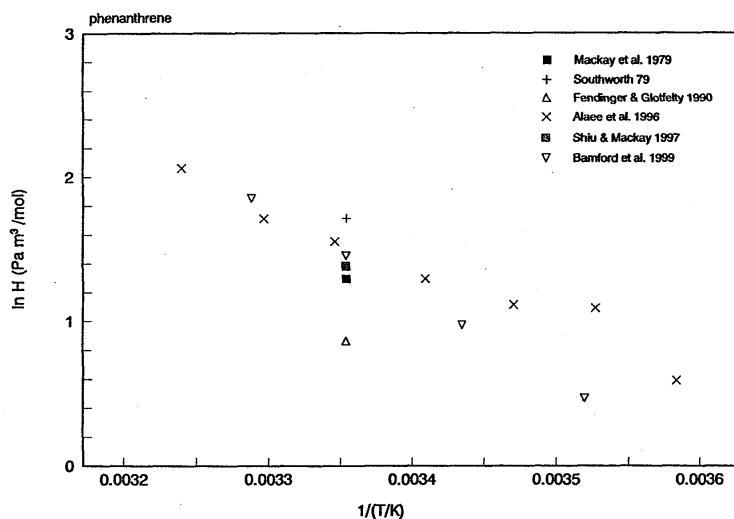


FIG. 38. Logarithm of Henry's law constant vs  $1/T$  for phenanthrene.

a series of handbooks [Mackay *et al.* (1992a), (1992b), (1993), (1995), (1997)] and the handbook on CD-ROM [Mackay *et al.*, (1998)]. These handbooks generally provide data for these chemicals only at 25 °C.

### 3. Temperature Dependence of the Properties

All three properties vary with temperature, the simplest general expression being the integrated Clapeyron–Clausius equation, or van't Hoff form expressing the effect of temperature on an equilibrium constant  $K_p$ ,

$$R \cdot \ln K_p = A_0 - B/T, \quad (7)$$

which can be rewritten as

$$\ln(x, p, H \dots) = A - \Delta H/RT, \quad (8)$$

where  $A_0$ ,  $B$ , and  $A$  are constants,  $\Delta H$  is the enthalpy of the phase change, i.e., evaporation from pure state for vapor pressure, dissolution from pure state into water for solubility, and for air–water transition in the case of Henry's law constant.

To obtain a better fit to experimental data by including more coefficients, the variation of these equilibrium constants with temperature can be expressed by [Clarke and Glew (1966)]

$$R \cdot \ln K_p(T) = A + B/T + C \cdot \ln T + DT + ET^2 + FT^3 + \dots, \quad (9)$$

where  $A$ ,  $B$ ,  $C$ ,  $D$ ,  $E$ , and  $F$  are constants.

There have been numerous approaches to describing the temperature dependence of these properties. For aqueous solubility, the most common expression is the van't Hoff equation of the form [Hildebrand *et al.*, (1970)]:

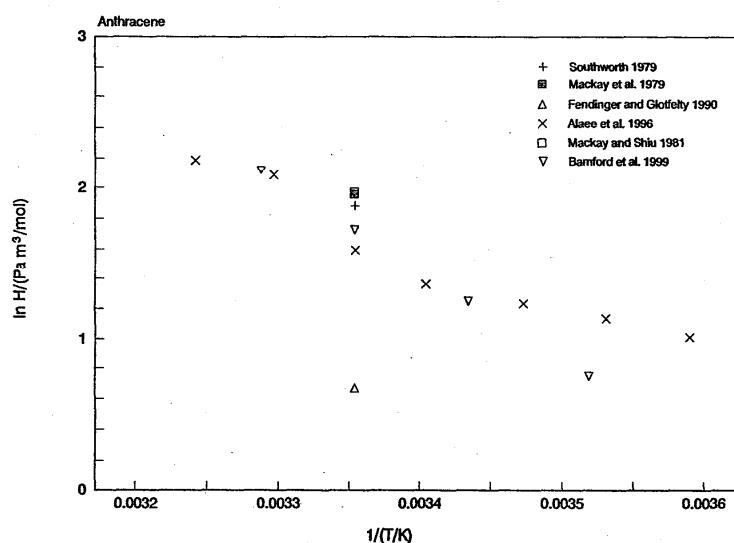


FIG. 39. Logarithm of Henry's law constant vs  $1/T$  for anthracene.

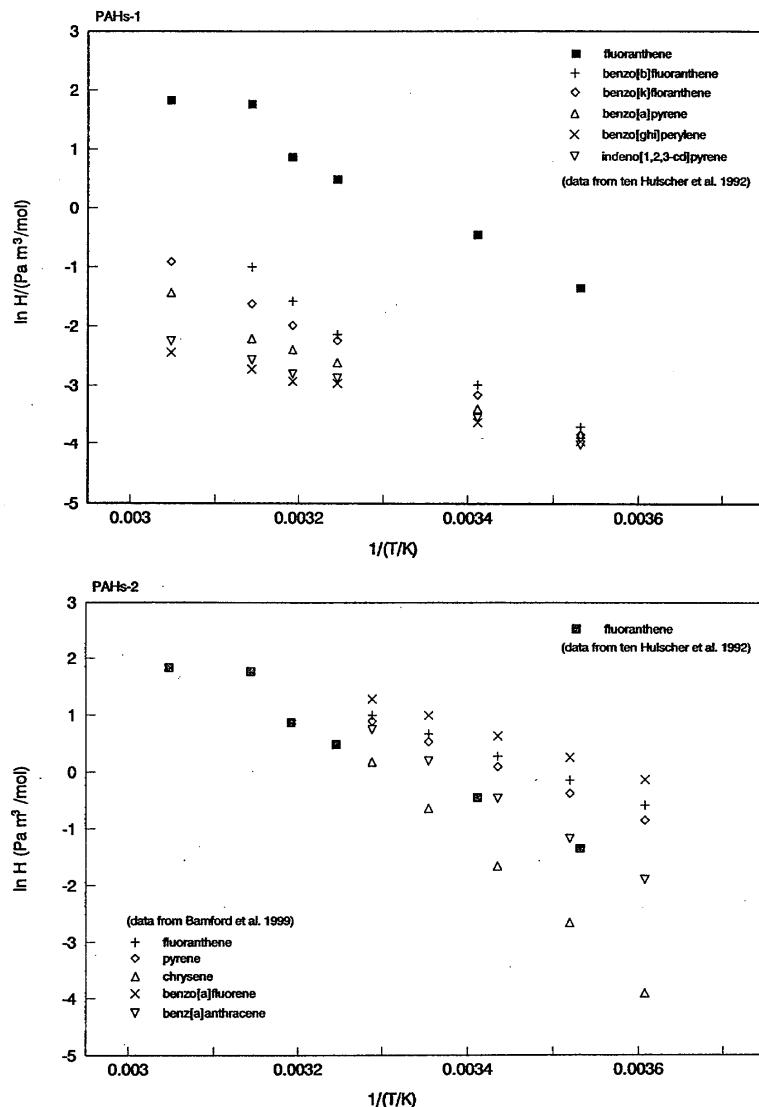


FIG. 40. Logarithm of Henry's law constant vs  $1/T$  for PAHs.

$$d(\ln x)/d(1/T) = -\Delta_{\text{sol}}H/R, \quad (10)$$

where  $x$  is the solubility in mole fraction units,  $T$  is the temperature in K,  $R$  is the gas constant, and  $\Delta_{\text{sol}}H$  is the enthalpy of solution of the solute. The enthalpy of solution can be considered as the sum of various contributions such as cavity formation and interactions between solute–solute or solute–solvent as discussed by Bohon and Claussen (1951), Arnold *et al.* (1958), Ueda *et al.* (1978), Owens *et al.* (1986), and many others. Assuming the enthalpy of solution is constant over a narrow temperature range, integration gives

$$\ln x = -\Delta_{\text{sol}}H/RT + C, \quad (11)$$

where  $C$  is a constant.

The relation between aqueous solubility and temperature is complicated because of the nature of the interactions between the solute and water structure. Not only does the en-

thalpy of solution vary with temperature, some liquid aromatic hydrocarbons display a minimum solubility corresponding to zero enthalpy of solution between 285 and 320 K. For example, benzene has a minimum solubility at 291 K [Bohon and Claussen (1951), Arnold *et al.* (1958), Shaw (1989a)] and alkylbenzenes display similar behavior [Shaw (1989a), (1989b), Owens (1986)]. As is illustrated later, solid aromatic hydrocarbons show a slight curvature in plots of logarithm of mole fraction solubility versus reciprocal absolute temperature. For narrow ranges in environmental temperatures, the enthalpy of solution may be assumed to be constant, and the linear van't Hoff plot of  $\ln x$  vs  $1/T$  is often used [Dickhut *et al.* (1989)]. Other relationships such as quadratic or cubic equations have been reported [May *et al.* (1978a), (1978b)], and polynomial series [Clarke and Glew (1966), May *et al.* (1983), Owens *et al.* (1986)] have been used when the data justify such treatment.



TABLE 2. Aqueous solubilities and reported equations for temperature dependence of aromatic hydrocarbons—Continued

Compound	$\Delta_{\text{sol}}H$ (kJ·mol <sup>-1</sup> )	t/°C	Reference	Solubility t/°C (S/g·m <sup>-3</sup> )	Method	Reference
Benzene (cont'd)			$\ln(f_2/x_2) = 12.4684 + 4.1683\theta - 4.097\theta^2 + 2.014\theta^3 + 14.04\theta^4 - 29.23\theta^5$ for temp range 5–69 °C, $f_2$ is the fugacity, $\theta = (T - 300)/100$			Franks <i>et al.</i> 1963
		25	1780	shake flask-GC	McAuliffe 1963, 1966	
		20	2100	polythermic method	Udovenko & Aleksandrova 1963	
		30	2270			
		40.5	2480			
		44.5	2590			
		56.5	2880			
		60	3000			
		65	3190			
		79.5	3730			
		25	1718	from vapor pressure	Taha <i>et al.</i> 1966	
		25	2170	vapor saturation-UV	Worley 1967	
		21	1740	shake flask-GC	Chey & Calder 1972	
		4	1710	shake flask-GC	Leinonen 1972	
		5	1737			
		5.4	1746			
		6.1	1735			
		7	1781			
		10.3	1748			
		13	1741			
		16	1730			
		19.1	1721			
		22.1	1739			
		25	1765			
		25	1765	shake flask-GC	Leinonen & Mackay 1973	
		0	1678	shake flask-GC	Polak & Lu 1973	
		25	1755			
		25	1740	shake flask-GC	Price 1973	
		55.3	3980			
		84.7	6468			
		25	1830	shake flask-spec.	Bradley <i>et al.</i> 1973	
		45	2160			
		55	2380			
		4.5	1840	shake flask-UV	Brown & Wasik 1974	
		6.3	1850			
		7.1	1810			
		9	1810			
		11.8	1770			
		12.1	1770			
		15.1	1790			
		17.9	1790			
		20.1	1760			
		25	1906	shake flask-GC	Vesala 1974	
		25	1769	shake flask-GC	Mackay <i>et al.</i> 1979	
		25	1780	shake flask-GC	Mackay & Shiu 1975	
		25	1760	shake flask-GC	Price 1976	
		25	1791	gen. col.-HPLC/UV	May <i>et al.</i> 1978b	
		0.2	1836	gen. col.-HPLC/UV	May 1977, 1980	
		6.2	1804			
		11	1799			
		14	1770			
		16.9	1762			
		18.6	1767			
		25	1791			
		25.8	1819			
			$S(\mu\text{g/kg}) = (1833 + 0.3166t - 0.6838 \cdot t^2 + 0.0247 \cdot t^3) \times 10^3$		May <i>et al.</i> 1978b	
			t in °C, correlation coeff. $r^2 = 0.9443$			
			$\log x = A/T^2 + B/T + C$ , for temp. range 0–55 °C		Ueda <i>et al.</i> 1978	
			$A = 424.544, B = -2955.82, C = 1.6606$			

## PROPERTIES OF ENVIRONMENTAL INTEREST

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TABLE 2. Aqueous solubilities and reported equations for temperature dependence of aromatic hydrocarbons—Continued

Compound	$\Delta_{\text{sol}}H$ (kJ·mol <sup>-1</sup> )	t/°C	Reference	t/°C	Solubility (S/g·m <sup>-3</sup> )	Method	Reference
Benzene (cont'd)		25		1769	shake flask-fluo.	Aquan-Yuen <i>et al.</i> 1979	
		10		1625	shake flask-spec.	Ben-Naim & Wiff 1979	
		20		1734			
		20		1790	shake flask-GC	Bittrich <i>et al.</i> 1979	
		40		2025			
		69		2442			
		25		1680	shake flask-GC	Ben-Naim & Wiff 1980	
		25		1750	shake flask-LSC	Banerjee <i>et al.</i> 1980	
		15		1540	vapor satn-spec.	Sanemasa <i>et al.</i> 1981	
		25		1610			
		35		1770			
		45		1870			
		5		1620	vapor satn-UV spec.	Sanemasa <i>et al.</i> 1982	
		15		1580			
		25		1620			
		35		1710			
		45		1800			
		20		1710	OECD methods	Schmidt-Bleek <i>et al.</i> 1982	
		25		1617	vapor satn-UV	Sanemasa <i>et al.</i> 1984	
		25		1878	shake flask-GC	Chiou <i>et al.</i> 1982, 1983	
		25		1789	gen. col.-HPLC/UV	Wasik <i>et al.</i> 1983	
		0.2		1837	gen. col.-HPLC/UV	May <i>et al.</i> 1983	
		6.2		1805			
		11		1800			
		14		1771			
		16.9		1763			
		18.6		1768			
		25		1792			
		25.8		1820			
					$R \cdot \ln x = -19.31/\theta + 2.1(1/\theta - 1/T) + 0.22[\theta/T - 1 - \ln(T/\theta)]$	May <i>et al.</i> 1983	
					eqn using thermodyn. parameters for process liq./solid→aq. at 25 °C, $\theta = 298.15$ K		
					$\ln x = -170.040 18 + 6922.912/T + 24.398 795 \ln T$ , for 313–373 K	Tsonopoulos & Wilson 1983	
					$\ln x = -442.923 52 + 15.357.083/T - 0.061 492 742 \cdot T + 70.543 13 \cdot \ln T$		
					$R \cdot \ln x = -3.63/\theta - 31.89(1/\theta - 1/T) + 0.30[\theta/T - 1 - \ln(\theta/T)]$	Owens <i>et al.</i> 1986	
					eq using thermodyn. parameters for process gas→aq. at 25 °C, $\theta = 298.15$ K		
					25      1810      shake flask-radiometric	Lo <i>et al.</i> 1986	
					25      1695      shake flask-GC	Keeley <i>et al.</i> 1988	
					25      1650      shake flask-GC	Coutant & Keigley 1988	
					$S(g/100 g) = 5.5773 - 4.6067 \times 10^{-2} \cdot T + 1.2504 \times 10^{-4} \cdot T^2 - 1.0489 \times 10^{-7} \cdot T^3$	Shaw 1989a	
					eq obtained from "best" lit. values, temp range 0–70 °C		
					20      1732      activity coeff.-GC	Cooling <i>et al.</i> 1992	
					30      1688		
					40      1712		
					50      1760		
					30      1840      equil. flow cell-GC	Chen & Wagner 1994a	
					40      2014		
					50      2213		
					60      2452		
					70      2713		
					80      3033		
					90      3472		
					100      4123		
					$\ln 1/x = -6.191 + 14.03(1/T_r) - 3.511(1/T_r^2)$ , temp range 30–100 °C		
					$T_r$ is the reduced temp, system temp $T$ divided by the critical temp $T_c$	Chen & Wagner 1994a,c	
					20      1803      shake flask-GC	Fredenslund <i>et al.</i> 1995	





TABLE 2. Aqueous solubilities and reported equations for temperature dependence of aromatic hydrocarbons—Continued

Compound	$\Delta_{\text{sol}}H$ (kJ·mol <sup>-1</sup> )	t/°C	Reference	t/°C	Solubility (g/m <sup>-3</sup> )	Method	Reference
Ethylbenzene (cont'd)				10	196.5	gen. col.-HPLC/UV	Owens <i>et al.</i> 1986
				14	192.4		
				17	188.6		
				18	183.2		
				19	178		
				20	188		
				21	183.2		
				22	181.9		
				23.5	186		
				25	192.3		
				25.8	186.2		
				28	185.5		
				30	188.7		
				35	193.1		
				40	204.8		
				45	211.4		
				$R \cdot \ln x = -3.7/\theta - 40.1(1/\theta - 1/T) + 0.33[\theta/T - 1 - \ln(\theta/T)]$			
				eq using thermodyn. parameters for process gas→aqueous, at 25 °C, $\theta = 298.15$ K			
				20	180	shake flask-GC	Burris & MacIntyre 1987
				25	172	shake flask-GC	Coutant & Keigley 1988
				30	170	equil. flow cell-GC	Chen & Wagner 1994c
				40	172		
				50	198		
				60	240		
				70	291		
				80	353		
				90	410		
				100	504		
				$\ln x = 11.59 - 20.52 \cdot T_r^{-1} + 4.750 \cdot T_r^2$ , for 303.15–373.15 K			
				$T_r$ is the reduced temp, i.e., system temp $T$ divided by critical temp $T_c$			
				recommended value at 25 °C: 160±20 g/m <sup>3</sup>			
o-Xylene							Chen & Wagner 1994c
				25	204	shake flask-UV	Andrews & Keefer 1949
				25	175	shake flask -GC	McAuliffe 1963
				0	142	shake flask -GC	Polak & Lu 1973
				25	213		
				25	170.5	shake flask -GC	Sutton & Calder 1975
				25	167	shake flask -GC	Price 1976
				25	167	shake flask -GC	Krzyzanowska & Szeliga '78
				10	212.4		
				20	240.0		
				25	221	gen. col.-HPLC/UV	Tewari <i>et al.</i> 1982b
				15	168	vapor extraction-spec.	Sanemasa <i>et al.</i> 1982
				25	179		
				35	198		
				45	214		
				25	176	shake flask-GC	Coutant & Keigley 1988
				recommended value at 25 °C: 170±10 g/m <sup>3</sup>			
m-Xylene	2.80	25	Bohon & Claussen 1951	25	102	shake flask-UV	Andrews & Keefer 1949
	-5.506	2		0.4	209	shake flask-UV spec.	Bohon & Claussen 1951
	-3.828	7		5.2	201		
	-1.59	12		14.9	192		
	0	17		21	196		
	1.22	22		25	196		
	1.99	27		25.6	196		
	3.92	32		30.3	198		
	8.87	37		34.9	203		
	2.49	25	Herington 1951	39.6	218		
	2.60	25	Sanemasa <i>et al.</i> 1982	0	196	shake flask-GC	Polak & Lu 1973
	2.90	25	Shaw 1989b	25	162		
	8.60	64–264	Pryor & Jentoft 1961	25	206	shake flask-spec.	Vesala 1974
	11.40	127–239	Chernoglazova & Simulin 1976	25	146	shake flask-GC	Sutton & Calder 1975
				20	160	synthetic method	Chernoglazova & Simulin 76
				40	220		
				70	380		



TABLE 2. Aqueous solubilities and reported equations for temperature dependence of aromatic hydrocarbons—Continued

Compound	$\Delta_{sol}H$ (kJ·mol <sup>-1</sup> )	t/°C	Reference	t/°C	Solubility (S/g·m <sup>-3</sup> )	Method	Reference
1,3,5-Trimethylbenzene (Mesitylene)	4.49	25	Chen & Wagner 1994c	25	20	residue volume	Booth & Everson 1948
				25	97	shake flask-UV	Andrews & Keefer 1950
				25	48.2	shake flask-GC	Sutton & Calder 1975
				15	45.6	vapor extraction-spec.	Sanemasa <i>et al.</i> 1982
				25	49.5		
				35	54.2		
				45	56.5		
				15	46	vapor extraction-spec.	Sanemasa <i>et al.</i> 1981
				25	50		
				35	54.9		
				45	58.9		
				30	64.0	equil. flow cell-GC	Chen & Wagner 1994c
				40	67.8		
				50	74.12		
				60	90.82		
				70	111		
				80	140		
				90	164		
				100	194		
			$\ln x = 11.33 - 20.64 \cdot T_r^{-1} + 4.630 \cdot T_r^{-2}$ ; for 303.15–373.15 K				Chen & Wagner 1994c
			$T_r$ is the reduced temp., system temp. $T$ divided by critical temp. $T_c$ recommended value at 25 °C: 50±5 g/m <sup>3</sup>				
n-Propylbenzene	-1.50 2.30 4.36	15 25 30	Gill <i>et al.</i> 1976	15 25 25	60.0 120 55.0	shake flask shake flask-turbidity shake flask-UV spec.	Föhner 1924 Stearns <i>et al.</i> 1947 Andrews & Keefer 1950
	3.70	25	Owens <i>et al.</i> 1986	25 25 25	120 60 70	shake flask-UV spec. shake flask shake flask-GC	Klevens 1950 Herman 1972 Krasnoshchekova, Gubergits 1975
				25	66.35	shake flask-spec.	Ben-Naim & Wiff 1979
				23	51.32	shake flask-HPLC/UV	DeVoe <i>et al.</i> 1981
				15	51.21	gen. col.-HPLC/UV	
				20	51.09		
				25	51.93		
				30	53.49		
				25	47.1	gen. col.-HPLC	Tewari <i>et al.</i> 1982a
				25	52.2	gen. col.-HPLC/UV; GC	Tewari <i>et al.</i> 1982b
				15	46.6	vapor extraction-spec.	Sanemasa <i>et al.</i> 1982
				25	51		
				35	55		
				45	64.1		
				25	45.2	vapor extraction-spec.	Sanemasa <i>et al.</i> 1984
				10	53.73	gen. col.-HPLC/UV	Owens <i>et al.</i> 1986
				15	52.29		
				20	54.33		
				25	53.25		
				30	52.53		
				35	56.61		
				40	63.95		
				45	66.59		
			$R \cdot \ln x = -2.14/\theta - 42.53(1/\theta - 1/T) + 0.52[\theta/T - 1 - \ln(\theta/T)]$ eq using thermodyn. parameters for process gas → aq. at 25 °C, $\theta = 298.15$ K recommended value at 25 °C: 52±5 g/m <sup>3</sup>				
Cumene	3.57 0 31.9	25 12 123.5	Glew & Robertson 1956	25 25	170 73.0	turbidity-photometer shake flask-UV	Stearns <i>et al.</i> 1947 Andrews & Keefer 1950
	5.1	25	Sanemasa <i>et al.</i> 1982	25	80.5	shake flask-spec.	Glew & Robertson 1956
				24.94	80.4	shake flask-spec.	Glew & Robertson 1956
				29.98	82.9		
				34.92	85.6		
				39.96	89.7		
				44.91	94.5		
				49.90	100.4		
				54.92	106.9		
				59.98	114.9		
				65.17	124.3		
				70.32	135.5		

TABLE 2. Aqueous solubilities and reported equations for temperature dependence of aromatic hydrocarbons—Continued

Compound	$\Delta_{\text{sol}}H$ (kJ·mol <sup>-1</sup> )	t/°C	Reference	t/°C	Solubility (S/g·m <sup>-3</sup> )	Method	Reference
Cumene (cont'd)				75.10	147.2		
				80.21	161.6		
				$\log x_2 = 4298.88/T + 24.6369 \cdot \log T - 105.044 \text{ 08}$ for temp range of 25–80 °C			Glew & Robertson 1956
				25	53	shake flask-GC	McAuliffe 1963
				25	50	shake flask-GC	McAuliffe 1966
				25	65.3	shake flask-GC	Sutton & Calder 1975
				25	48.3	shake flask-GC	Price 1976
				25	48.3	shake flask-GC	Krzyzanowska & Szeliga 1978
				15	59.5	vapor extraction-spec.	Sanemasa <i>et al.</i> 1982
				25	61.5		
				35	68.7		
				45	77.5		
				recommended value at 25 °C: 50±5 g/m <sup>3</sup>			
n-Butylbenzene	6.6 1.29	25 25	Owens <i>et al.</i> 1986 Chen & Wagner 1994c	25 25 25 25 25 25 7 10 12.5 15 17.5 20 25 30 35 40 45	12.61 50.5 17.71 11.8 13.82 13.8 13.34 12.98 13.14 12.96 13.14 13.66 13.76 14.57 15.39 16.56 18.94	shake flask-UV shake flask-UV shake flask-GC shake flask-GC gen. col.-HPLC, GC gen. col.-HPLC/UV gen. col.-HPLC	Andrews & Keefer 1950 Klevens 1950 Massadie & King 1973 Sutton & Calder 1975 Tewari <i>et al.</i> 1982b Wasik <i>et al.</i> 1983 Owens <i>et al.</i> 1986
				$R \cdot \ln x = -1.42/\theta - 44.15(1/\theta - 1/T) + 0.61[\theta/T - 1 - \ln(\theta/T)]$ eq using thermodyn. parameters for process gas→aq. at 25 °C, $\theta = 298.15 \text{ K}$			
				20 30 40 50 60 70 80 90 100	13.3 16.7 17.82 20.3 26.9 32.06 47.72 61.14 83.5	shake flask-GC equil. flow cell-GC	Burris & MacIntyre 1987 Chen & Wagner 1994c
				$\ln x = 26.26 - 35.26 \cdot T_r^{-1} + 7.905 \cdot T_r^{-2}$ ; for 303.15–373.15 K recommended value at 25 °C: 13.8±1.2 g/m <sup>3</sup>			Chen & Wagner 1994c
1,2-Diethylbenzene				10 20	71.3 71.3	shake flask-spec.	Ben-Naim & Wiff 1979
				recommended value at 25 °C			
1,4-Diethylbenzene				10 20	24.83 24.83	shake flask-spec.	Ben-Naim & Wiff 1979
				recommended value at 25 °C			
n-Pentylbenzene	6.5	25	Owens <i>et al.</i> 1986	25 25 7 10 12.5 15 17.5 20 25 30 35 40 45 45	10.5 3.84 3.48 3.18 3.44 3.19 3.43 3.18 3.37 3.61 3.92 4.25 4.69 4.69	shake flask-UV gen. col.-HPLC/UV gen. col.-HPLC	Andrews & Keefer 1950 Tewari <i>et al.</i> 1982b Owens <i>et al.</i> 1986

TABLE 2. Aqueous solubilities and reported equations for temperature dependence of aromatic hydrocarbons—Continued

Compound	$\Delta_{\text{sol}}H$ (kJ·mol <sup>-1</sup> )	t/°C	Reference	t/°C	Solubility (S/g·m <sup>-3</sup> )	Method	Reference
n-Pentylbenzene (cont'd)					$R \cdot \ln x = -0.67/\theta - 49.47(1/\theta - 1/T) + 0.76[\theta/T - 1 - \ln(\theta/T)]$ eq using thermodyn. parameters for process gas→aq. at 25 °C, $\theta = 298.15$ K recommended value at 25 °C: $3.85 \pm 0.30$ g/m <sup>3</sup>		
Hexylbenzene	7.6	25	May <i>et al.</i> 1983	25	17.02	shake flask-spec.	Ben-Naim & Wiff 1979
	8.00	25	Owens <i>et al.</i> 1986	25	1.018	gen. col.-HPLC/UV	Tewari <i>et al.</i> 1982b
				5	0.921	gen. col.-HPLC	May <i>et al.</i> 1983
				6	0.921		
				8	0.920		
				9	0.906		
				10	0.904		
				11	0.928		
				12	0.930		
				13	0.920		
				14	0.925		
				15	0.908		
				16	0.919		
				17	0.910		
				18	0.921		
				19	0.943		
				20	0.949		
				21	0.956		
				22	0.953		
				23	0.983		
				24	0.995		
				25	0.999		
				26	0.999		
				27	0.999		
				29	1.016		
				$R \cdot \ln x = -39.7/\theta + 7.6(1/\theta - 1/T) + 0.51[\theta/T - 1 + \ln(T/\theta)]$ eq using thermodyn. parameters for process liq/solid→aq. at 25 °C, $\theta = 298.15$ K			
				$R \cdot \ln x = -0.05/\theta - 52.34(1/\theta - 1/T) + 0.48[\theta/T - 1 - \ln(\theta/T)]$ eq using thermodyn. parameters for process gas→aq. at 25 °C, $\theta = 298.15$ K		given by Owens <i>et al.</i> 1986	
				7	0.833	gen. col.-HPLC	Owens <i>et al.</i> 1986
				10	0.836		
				15	0.826		
				20	0.951		
				25	0.902		
				30	0.996		
				35	1.069		
				40	1.069		
				45	1.298		
				$R \cdot \ln x = -0.21/\theta - 52.7(1/\theta - 1/T) + 0.61[\theta/T - 1 - \ln(\theta/T)]$ eq using thermodyn. parameters for process gas→aq. at 25 °C, $\theta = 298.15$ K			
				recommended value at 25 °C: $1.02 \pm 0.10$ g/m <sup>3</sup>			
Styrene				7	290	shake flask-titration	Lane 1946
				24	330		
				32	360		
				40	400		
				51	450		
				15	250	shake flask-cloud point	Lane 1946
				25	310		
				44	400		
				49	450		
				56	500		
				65	580		
				60.3	960	shake flask turbidity	Fordyce & Chapin 1947
				25	220	shake flask	Fritelte & Hohenstein 1948
				25	300	shake flask-UV	Andrews & Keefer 1950
				25	160	shake flask-HPLC/UV	Banerjee <i>et al.</i> 1980
				recommended value at 25 °C: $320 \pm 20$ g/m <sup>3</sup>			
Naphthalene	4.14	2	Bohon & Claussen 1951	25	30	shake flask-gravimetric	Hilpert 1916
	5.77	7		25	31.5	shake flask-UV	Andrews & Keefer 1949
	7.24	12		25	12.5	shake flask-UV	Klevens 1950
	8.49	17		25	34.4	shake flask-UV spec.	Bohon & Claussen 1951
	10.17	22		0	13.74		
	12.80	27		0.4	13.74		
	14.23	32		0.5	13.85		

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TABLE 2. Aqueous solubilities and reported equations for temperature dependence of aromatic hydrocarbons—Continued

Compound	$\Delta_{\text{sol}}H$ (kJ·mol <sup>-1</sup> )	t/°C	Reference	t/°C	Solubility (g/m <sup>3</sup> )	Method	Reference
Naphthalene (cont'd)	15.69	37		0.9	14.59		
	18.74	42		1.9	15.03		
	29.9	25		9.4	19.62		
	29.9	25	Wauchope & Haque 1972	10	19.42		
	18.0	10–30	Schwarz & Wasik 1976	14.9	23.43		
	22.1	8–32	Schwarz 1977	15.9	24.56		
	26.4	5–30	May <i>et al.</i> 1978b	19.3	28.05		
	27.4	25	May <i>et al.</i> 1983	25.6	36.6		
				30.1	42.97		
				30.2	43.87		
				35.2	54.45		
				36	54.81		
				42.8	73.49		
				25	20.4	shake flask	Sahyun 1966
				25	33.47	shake flask-GC	Gordon & Thorne 1967
				20	38.4	shake flask-UV	Eisenbrand & Baumann 1970
				0	13.7	shake flask-GC	Wauchope & Getzen 1972
				22.2	28.3		
				24.5	30.7		
				25	31.2		
				29.9	37.3		
				30.3	37.8		
				34.5	44.3		
				39.3	53.3		
				40.1	55		
				44.7	66.2		
				50	82.4		
				50.2	83.1		
				55.6	105		
				64.5	156		
				73.4	239		
				75	258		
	$R \cdot \ln x = -8.69/T + (0.000408)(T - 291.15)^2 - 13.4 + 139 \cdot T$						
	for temp. range 29.9–73.4 °C						
				25	32.17	shake flask-UV	Vesala 1974
				25	31.3	shake flask-GC	Eganhouse & Calder 1975
				25	22.00	shake flask-fluo.	Schwarz & Wasik 1976
				25	31.7	shake flask-fluo.	Mackay & Shiu 1977
				10	18.59	shake flask-fluo.	Schwarz & Wasik 1977
				12	20.13		
				15	22.56		
				16	23.59		
				18	24.36		
				19	26.92		
				25	30.0		
				26	34.36		
				8.4	17.95	shake flask-fluo.	Schwarz 1977
				11.1	19.1		
				14	21.2		
				17.5	24.1		
				20.2	26.54		
				23.2	28.46		
				25	30.25		
				26.3	31.79		
				29.2	34.36		
				31.8	36.28		
				25	31.69	gen. col.-HPLC/UV	May <i>et al.</i> 1978b
				8.20	16.92	gen. col.-HPLC/UV	May 1980; May <i>et al.</i> 1983
				11.50	19.25		
				13.40	20.39		
				15.10	21.50		

TABLE 2. Aqueous solubilities and reported equations for temperature dependence of aromatic hydrocarbons—Continued

Compound	$\Delta_{\text{sol}}H$ (kJ·mol <sup>-1</sup> )	t/°C	Reference	t/°C	Solubility (S/g·m <sup>-3</sup> )	Method	Reference
Naphthalene (cont'd)					19.30		25.81
		23.40			29.50		
		25.00			31.94		
		27.00			34.18		
			$S \text{ (mg/kg)} = 13.66 + 0.2409 \cdot t + 0.0189 \cdot t^2, t \text{ in } ^\circ\text{C}$				May 1977, 1980
			$R \cdot \ln x = -30.55/\theta + 28.7/(1/\theta - 1/T) + 0.31[\theta/T - 1 - \ln(\theta/T)], T \text{ in K}$				May <i>et al.</i> 1983
			eq using thermodyn. parameters for process liq/solid→aq. at 25 °C, $\theta = 298.15 \text{ K}$				
		25		30.64	gen. col.-HPLC/UV		Wasik <i>et al.</i> 1983
		25		32.9	gen. col.-HPLC/fluor.		Walters & Luthy 1984
		25		31.1	shake flask-UV		Bennett & Canady 1984
		1.90		19.20			
		10.70		17.20			
		15.40		21.66			
		21.70		26.74			
		25.20		30.75			
		30.70		40.12			
		35.10		46.36			
		39.30		54.85			
		44.90		68.97			
			$\ln x = -1767.4601/RT + (17.952/0.9R) \cdot \ln T + 1, \text{ for temp. } 2-45 \text{ }^\circ\text{C}$				Bennett & Canady 1984
		25		30.6	shake flask-HPLC/UV		Fu & Luthy 1985
		25		30.1	vapor saturation-UV		Akiyoshi <i>et al.</i> 1987
		25		31.3	gen. col.-HPLC/UV		Billington <i>et al.</i> 1988
		25		31.9	gen. col.-HPLC/UV		Billington <i>et al.</i> 1988
		25		31.3	shake flask-HPLC/UV		Dickhut <i>et al.</i> 1989
		5		12.30	shake flask-UV spec.		Perez-Tejeda <i>et al.</i> 1990
		10		20.25			
		15		24.35			
		20		28.71			
		25		33.71			
		30		41.53			
		35		47.55			
		40		55.75			
			$\log(S/\text{mol} \cdot \text{dm}^3) = -31.24 - 143.5/T + 4.772 \cdot \ln T, \text{ temp range } 5-40 \text{ }^\circ\text{C}$				Perez-Tejeda <i>et al.</i> 1990
		25		30	shake flask-UV/fluor.		Pinal <i>et al.</i> 1991
		25		30.6	gen. col.-HPLC		Vadas <i>et al.</i> 1991
		25		30.6	gen. col.-GC		Vadas <i>et al.</i> 1991
		25		33.9	gen. col.-GC		Coyle <i>et al.</i> 1997
		25		34.8	gen. col.-HPLC/fluor.		De Maagd <i>et al.</i> 1998
		25		36.0(a)	supercritical water extr.		Miller & Hawthorne 1998
			recommended value at 25 °C: $31.5 \pm 2.0 \text{ g/m}^3$				
1-Methylnaphthalene	19.1	Schwarz 1977	25	25.8	shake flask-GC	Eganhouse & Calder 1976	
			25	28.5	shake flask-fluor.	Mackay & Shiu 1977	
			8.6	19.91	shake flask-fluor.	Schwarz 1977	
			14	22.61			
			17.1	22.89			
			20	25.31			
			23	27.59			
			25	30.0			
			26.1	30.43			
			29.2	33.28			
			31.7	36.26			
			10	22.75	shake flask-fluor.	Schwarz & Wasik 1977	
			14	28.44			
			20	28.44			
			25	29.86			
			25	31.7	gen. col.-HPLC	Wasik <i>et al.</i> 1983	
			20	30.2	shake flask-GC	Burris & MacIntyre 1986, 1987	
			70	87.9			
			recommended value at 25 °C: $28.0 \pm 2.0 \text{ g/m}^3$				
1-Ethynaphthalene	13.1	Schwarz 1977	25	10.7	shake flask-fluor.	Mackay & Shiu 1977	

TABLE 2. Aqueous solubilities and reported equations for temperature dependence of aromatic hydrocarbons—Continued

Compound	$\Delta_{\text{sol}}H$ (kJ·mol <sup>-1</sup> )	t/°C	Reference	t/°C	Solubility (S/g·m <sup>-3</sup> )	Method	Reference
4 Ethylnaphthalene (cont'd)				8.6	8.124	shake flask fluo.	Schwarz 1977
				11.1	8.124		
				14	8.28		
				17.1	8.593		
				20	8.436		
				23	8.593		
				25	9.999		
				26.1	9.842		
				31.7	11.72	shake flask-spec.	Schwarz & Wasik 1977
				10	8.1		
				14	8.1		
				20	10.0		
				25	10		
				25	11.58	gen. col.-HPLC	Wasik <i>et al.</i> 1983
			recommended value at 25 °C: 10.0±1.0 g/m <sup>3</sup>				
Biphenyl	7.03	2	Bohon & Claussen 1951	25	5.94	shake flask-UV	Andrews & Keefer 1949
	10.12	7		0.4	2.83	shake flask-UV	Bohon & Claussen 1951
	10.88	12		2.4	2.97		
	12.55	17		5.2	3.38		
	13.43	22		7.6	3.64		
	15.02	27		10	4.06		
	18.58	32		12.6	4.51		
	21.42	37		14.9	5.11		
	21.09	42		15.9	5.27		
	33	25	Dickhut <i>et al.</i> 1986	25	7.48		
				25.6	7.78		
				30.1	9.64		
				30.4	9.58		
				33.3	11		
				34.9	11.9		
				36	12.5		
				42.8	17.2		
				0	2.64	shake flask-UV	Wauchope & Getzen 1972
				24.8	7.13		
				25	7.08		
				29.9	8.77		
				30.3	8.55		
				38.4	13.2		
				40.1	13.1		
				47.5	18.8		
				50.1	20.6		
				50.2	20.7		
				54.7	28.3		
				59.2	36.4		
				60.5	40.4		
				64.5	43.7		
				25	7.571	shake flask-spec.	Vesala 1974
				25	3.47	shake flask-GC/FID	Eganhouse & Calder 1976
				25	7.00	shake flask-fluo.	Mackay & Shiu 1977
				25	8.50	nephelometry	Hollifield 1979
				25	6.03	shake flask-HPLC	Banerjee <i>et al.</i> 1980
				25	6.71	gen. col.-GC	Miller <i>et al.</i> 1984
				25	7.05	vapor saturation-UV	Akiyoshi <i>et al.</i> 1987
				25	6.50	shake flask-GC	Stucki & Alexander 1987
				25	7.20	gen. col.-HPLC/UV	Billington <i>et al.</i> 1988
				25	6.99	gen. col.-GC	Coyle <i>et al.</i> 1997
			recommended value at 25 °C: 7.2±0.50 g/m <sup>3</sup>				
4-Methylbiphenyl	27.5		Doucette and Andren 1988	4.9	1.83	generator col.-GC	Doucette & Andren 1988
				25	4.05		
				40	7.03		
			$\log x = -1.436/T - 1.541$				
			$c/(M\cdot L^{-1}) = 9.18 \times 10^{-6} \exp[0.038 \cdot (t/^\circ C)]$				
			recommended value at 25 °C: 4.05 g/m <sup>3</sup>				
4,4'-Dimethylbiphenyl	36.6		Doucette and Andren 1988	4.0	0.0678	generator col.-GC	Doucette & Andren 1988
				25	0.175		
							Doucette & Andren 1988
							Doucette 1985







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TABLE 2. Aqueous solubilities and reported equations for temperature dependence of aromatic hydrocarbons

Compound	$\Delta_{sol}H$ (kJ·mol <sup>-1</sup> )	t/°C	Reference	Solubility t/°C (S/g·m <sup>-3</sup> )	Method	Reference
2-Methylanthracene (cont'd)				18.3 0.0145 23.1 0.0191 27 0.0242 31.1 0.0321		
				$S(\mu\text{g/kg}) = 2.78 + 0.818 \cdot t - 0.0306 \cdot t^2 + 0.0011 \cdot t^3$ , t in °C $R \cdot \ln x = -49.61/\theta + 45.5(1/\theta - 1/T) + 0.018[\theta/T - 1 - \ln(\theta/T)]$		May 1977; May <i>et al.</i> 1978 May <i>et al.</i> 1983
				eq using thermodyn. parameters for process liq./solid→aq. at 25 °C, $\theta = 298.15\text{ K}$ recommended value at 25 °C: $0.030 \pm 0.010\text{ g/m}^3$		
Pyrene						
	30.5	Wauchope & Haque 1972	27	0.165	shake flask-nephelometry	Davis <i>et al.</i> 1942
	47.7	8–32 Schwarz 1977	25	0.175	shake flask-UV	Klevens 1950
	35.4	5–30 May <i>et al.</i> 1978b	25	1.56	shake flask UV/fluor.	Barone <i>et al.</i> 1967
			25	0.105		Eisenbrand & Baumann 1970
			0	0.049	shake flask-UV	Wauchope & Getzen 1972
			22.2	0.129		
			25	0.148		
			34.5	0.228		
			44.7	0.397		
			50.1	0.558		
			55.6	0.75		
			56	0.74		
			60.7	0.96		
			65.2	1.27		
			71.9	1.83		
			74.7	2.21		
				$R \cdot \ln x = -3.66/T + (0.000408)(T - 291.15)^2 - 38.1 + 478 \cdot T$ for temp range 22.2–74.4 °C		
			25	0.135	shake flask-fluor.	Mackay & Shiu 1977
			12.2	0.055	shake flask-fluor.	Schwarz 1977
			15.5	0.069		
			17.4	0.079		
			20.3	0.092		
			23	0.117		
			23.3	0.118		
			25	0.129		
			26.2	0.144		
			26.7	0.145		
			28.5	0.164		
			31.3	0.188		
			25	0.132	gen. col.-HPLC	May <i>et al.</i> 1978b
			29	0.162		
			4.7	0.0492	gen. col.-HPLC	May 1977; May <i>et al.</i> 1983
			9.5	0.0586		
			14	0.0721		
			18.7	0.0934		
			21.2	0.1091		
			25.5	0.1361		
			29.9	0.1701		
				$S(\mu\text{g/kg}) = 50.2 - 1.051 \cdot t + 0.2007 \cdot t^2 - 0.0011 \cdot t^3$ , t in °C $R \cdot \ln x = -45.29/\theta + 41.6(1/\theta - 1/T) + 0.034[\theta/T - 1 - \ln(\theta/T)]$		May 1977, 1980, May <i>et al.</i> 1978b May <i>et al.</i> 1983
				eq using thermodyn. parameters for process liq./solid→aq. at 25 °C, $\theta = 298.15\text{ K}$		
			25	0.032	shake flask-nephelometry	Hollifield 1979
			25	0.130	shake flask-GC	Rossi & Thomas 1981
			25	0.118	gen. col.-HPLC	Billington <i>et al.</i> 1988
			25	0.107	gen. col.-HPLC/fluor.	Vadas <i>et al.</i> 1991
				recommended value at 25 °C: $0.132 \pm 0.02\text{ g/m}^3$		
Fluoranthene	39.8	5–30 May <i>et al.</i> 1978b	27	0.240	shake flask-nephelometry	Davis <i>et al.</i> 1942
			25	0.260	shake flask-UV	Klevens 1950
			20	0.240	shake flask-UV	Eisenbrand & Baumann 1970

TABLE 2. Aqueous solubilities and reported equations for temperature dependence of aromatic hydrocarbons—Continued

Compound	$\Delta_{\text{sol}}H$ (kJ·mol <sup>-1</sup> )	t/°C	Reference	t/°C	Solubility (g/g·m <sup>-3</sup> )	Method	Reference
Fluoranthene (cont'd)				25	0.236	shake flask-UV	Schwarz & Wasik 1976
				25	0.260	shake flask-fluo.	Mackay & Shiu 1977
				25	0.206	gen. col.-HPLC	May <i>et al.</i> 1978b
				29	0.264	gen. col.-HPLC	May <i>et al.</i> 1978b
				25	0.120	shake flask-nephelometry	Hollifield 1979
				20	0.184	shake flask-fluo.	Hanshimoto <i>et al.</i> 1982
				20	0.190	gen. col.-fluorescence	Hanshimoto <i>et al.</i> 1982
				20	0.20	OECD methods	Schmidt-Bleek <i>et al.</i> 1982
				8.1	0.0821	gen. col.-HPLC	May 1977; May <i>et al.</i> 1983
				13.2	0.1071		
				19.7	0.1484		
				24.6	0.2028		
				29.9	0.2796		
				$S(\mu\text{g/kg}) = 50.4 + 4.322 \cdot t - 0.1047 \cdot t^2 + 0.0072 \cdot t^3$ , $t$ in °C			May 1977, 1980, May <i>et al.</i> 1978b
				$R \cdot \ln x = -44.16/\theta + 45.0(1/\theta - 1/T) + 0.022[\theta/T - 1 - \ln(\theta/T)]$			May <i>et al.</i> 1983
				eq using thermodyn. parameters for liq./solid→aq. process at 25 °C, $\theta = 298.15$ K			
				25	0.199	gen. col.-HPLC/fluo.	Waters & Luthy 1984
				25	0.283	vapor saturation-UV	Akiyoshi <i>et al.</i> 1987
				15	0.133	gen. col.-HPLC/fluo.	Kishi & Hashimoto 1989
				25	0.222		
				15	0.275	gen. col.-HPLC/fluo.	Kishi & Hashimoto 1989
				25	0.373		
				20	0.166	shake flask-fluo.	Kishi & Hashimoto 1989
				25	0.265	shake flask-HPLC/fluo.	Pinal <i>et al.</i> 1991
				25	0.177	gen. col.-HPLC/fluo.	Vadas <i>et al.</i> 1991
				25	0.248	gen. col.-HPLC/UV	Yu & Xu 1993
				25	0.207	gen. col.-HPLC/fluo.	De Maagd <i>et al.</i> 1998
				recommended value at 25 °C: 0.260±0.060 g/m <sup>3</sup>			
Chrysene	41.3	5–30	May <i>et al.</i> 1978b	27	0.001	shake flask-nephelometry	Davis <i>et al.</i> 1942
				25	0.006	shake flask-UV	Klevens 1950
				25	0.002	shake flask-fluo.	Mackay & Shiu 1977
				25	0.0018	gen. col.-HPLC	May <i>et al.</i> 1978b
				29	0.0022		
				6.5	0.00071	gen. col.-HPLC	May 1977; May <i>et al.</i> 1983
				11	0.00080		
				20.4	0.00140		
				24	0.00168		
				25.3	0.00189		
				28.7	0.00221		
				$S(\mu\text{g/kg}) = 0.609 - 0.0144 \cdot t + 0.0024 \cdot t^2$ , $t$ in °C			May <i>et al.</i> 1978b
				$R \cdot \ln x = -56.21/\theta + 45.4(1/\theta - 1/T) + 0.054[\theta/T - 1 - \ln(\theta/T)]$			May <i>et al.</i> 1983
				eq using thermodyn. parameters for process liq./solid→aq. at 25 °C, $\theta = 298.15$ K			
				25	0.017	shake flask-nephelometry	Hollifield 1979
				25	0.00107	gen. col.-HPLC	Billington <i>et al.</i> 1988
				25	0.0012	gen. col.-HPLC	Billington <i>et al.</i> 1988
				25	0.0016	gen. col.-HPLC/fluo.	Vadas <i>et al.</i> 1991
				23	0.00079	shake flask-HPLC	Li & Yalkowsky 1994
				25	0.0015	gen. col.-HPLC/fluo.	De Maagd <i>et al.</i> 1998
				recommended value at 25 °C: 0.002±0.001 g/m <sup>3</sup>			
Benz[ <i>a</i> ]anthracene				27	0.011	shake flask-nephelometry	Davis <i>et al.</i> 1942
				25	0.01	shake flask-UV	Klevens 1950
				25	0.014	shake flask-fluo.	Mackay & Shiu 1977
				25	0.0094	gen. col.-HPLC	May <i>et al.</i> 1978b
				29	0.0122	gen. col.-HPLC	May <i>et al.</i> 1978b
				6.9	0.00299	gen. col.-HPLC	May 1977, 1980
				10.7	0.00378		
				14.3	0.00479		
				19.3	0.00277		

TABLE 2. Aqueous solubilities and reported equations for temperature dependence of aromatic hydrocarbons—Continued

Compound	$\Delta_{sol}H$ (kJ·mol <sup>-1</sup> )	t/°C	Reference	t/°C	Solubility (S/g·m <sup>-3</sup> )	Method	Reference
B[a]A (cont'd)		23.1		23.1	0.008 37		
		29.7		29.7	0.0127		
			$S(\mu\text{g/kg}) = 1.74 + 0.1897 \cdot t - 0.0031 \cdot t^2 + 0.0003 \cdot t^3$ , $t$ in °C				May <i>et al.</i> 1978b
			$R \cdot \ln x = -52.21/\theta + 50.0(1/\theta - 1/T) + 0.038[\theta/T - 1 - \ln(\theta/T)]$				May <i>et al.</i> 1983
			eq using thermodyn. parameters for process liq./solid→aq. at 25 °C, $\theta = 298.15$ K				
		25		0.044	shake flask-nephelometry	Hollifield 1979	
		6.9		0.002 99	gen. col.-HPLC	May <i>et al.</i> 1983	
		10.7		0.003 78			
		11.1		0.003 61			
		14.7		0.004 79			
		18.1		0.005 58			
		19.3		0.006 34			
		23.6		0.008 01			
		23.1		0.008 38			
		25		0.008 62			
		29.5		0.012 41			
		29.1		0.012 71			
		25		0.009 4	gen. col.-HPLC	Billington <i>et al.</i> 1988	
		25		0.014 6	shake flask-HPLC	Haines & Sandler 1995	
		25		0.013 0	gen. col.-HPLC/fluo.	De Maagd <i>et al.</i> 1998	
			recommended value at 25 °C: 0.011 ± 0.002 g/m <sup>3</sup>				
Tripheylene		27		0.038	nephelometry	Davis <i>et al.</i> 1942	
		25		0.043	shake flask-UV	Klevens 1950	
		25		0.057	shake flask-UV	Eisenbrand & Baumann 1970	
		25		0.043	shake flask-fluo.	Mackay & Shiu 1977	
		8		0.002 99	gen. col.-HPLC	May 1977; May <i>et al.</i> 1983	
		12		0.003 03			
		14.8		0.003 39			
		20.5		0.004 89			
		27.3		0.007 70			
		28.2		0.008 12			
			$S(\mu\text{g/kg}) = 4.89 - 0.4250 \cdot t + 0.0250 \cdot t^2 - 0.0002 \cdot t^3$ , $t$ in °C				May 1977, 1980
			$R \cdot \ln x = -53.09/\theta + 56.9(1/\theta - 1/T) + 0.063[\theta/T - 1 - \ln(\theta/T)]$				May <i>et al.</i> 1983
			eq using thermodyn. parameters for process liq./solid→aq. at 25 °C, $\theta = 298.15$ K				
		25		0.006 62	gen. col.-HPLC	May 1977, 1980	
		25		0.041 1	vapor saturation-UV	Akiyoshi <i>et al.</i> 1987	
			recommended value at 25 °C: 0.043 ± 0.005 g/m <sup>3</sup>				
Benzo[a]pyrene		27		0.004	shake flask-nephelometry	Davis <i>et al.</i> 1942	
		25		0.0043	shake flask-UV/fluo.	Barone <i>et al.</i> 1967	
		25		0.0038	shake flask-fluo.	Mackay & Shiu 1977	
		10		0.000 56	gen. col.-HPLC/UV	May <i>et al.</i> 1983	
		15		0.000 80			
		20		0.001 14			
		25		0.001 62			
		30		0.002 29			
			$R \cdot \ln x = -56.71/\theta + 50.3(1/\theta - 1/T) + 0.013[\theta/T - 1 - \ln(\theta/T)]$				
			eq using thermodyn. parameters for process liq./solid→aq. at 25 °C, $\theta = 298.15$ K				
		25		0.001 2	gen. col.-HPLC	Wise <i>et al.</i> 1981	
		25		0.001 6	gen. col.-HPLC/UV	Billington <i>et al.</i> 1988	
		25		0.004 72	shake flask-fluo.	Haines & Sandler 1995	
		23		0.003 2	shake flask-HPLC	Li & Yalkowsky 1994	
		25		0.001 82	gen. col.-HPLC/fluo.	De Maagd <i>et al.</i> 1998	
			recommended value at 25 °C: 0.0030 ± 0.002 g/m <sup>3</sup>				
Benzo[e]pyrene	25.6	8–32	Schwarz 1977	25	0.007 32	shake flask-UV/fluo.	Barone <i>et al.</i> 1967
				8.6	0.003 25	shake flask-fluo.	Schwarz 1977
				14	0.003 58		
				17	0.004 44		
				17.5	0.003 94		

TABLE 2. Aqueous solubilities and reported equations for temperature dependence of aromatic hydrocarbons—Continued

Compound	$\Delta_{\text{sol}}H$ (kJ·mol <sup>-1</sup> )	t/°C	Reference	t/°C	Solubility (S/g·m <sup>-3</sup> )	Method	Reference
Dibenz[ <i>a,h</i> ]anthracene		20		20	0.004 59		
		20.2		20.2	0.004 79		
		23.2		23.2	0.005 35		
		23		23	0.005 07		
		29.2		29.2	0.006 38		
		31.7		31.7	0.006 81		
		recommended value at 25 °C: 0.005±0.002 g/m <sup>3</sup>					
		27		27	0.0005	shake flask-nephelometry	Davis <i>et al.</i> 1942
		25		25	0.0006	shake flask-UV	Klevens 1950
		25		25	0.0025	shake flask-LSC	Means <i>et al.</i> 1980
		recommended value at 25 °C: 0.0006±0.0002 g/m <sup>3</sup>					

*S* - solubility in g·m<sup>-3</sup>, mg·L<sup>-1</sup>, or  $\mu\text{g}\cdot\text{kg}^{-1}$ ; *c* in mol·m<sup>-3</sup>; *x* is mole fraction

*T* - temperature in K; *t* in °C;  $\theta$  in K

*R* - gas constant

IR - infrared spectroscopy

UV - UV spectrophotometry

GC - gas chromatography

GC/FID - GC analysis with flame ionization detector

GC/ECD - GC analysis with electron capture detector

HPLC - high pressure liquid chromatography, HPLC/UV - HPLC with UV detector

fluo. - fluorescence, HPLC/fluo. - HPLC with fluorescence detector

LSC - liquid scintillation counting

gen. col. - generator column technique for preparation of saturated aqueous solution

*a* only values determined at 1 atm. pressure for using are reported

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TABLE 3. Vapor pressures and reported equations for temperature dependence of aromatic hydrocarbons

Compound	t/°C, T/K or temp range	Vapor pressure or reported equations: ( $\mu^{\circ}$ /Pa)	Method	Reference
Benzene	0	3509	mercury/oil manometer	Stuckey & Saylor 1940
	10	6040		
	20	9960		
	30	15 800		
	40	24 240		
	50	36 050		
	0.97–53.49 °C	$\log(p/\text{mmHg}) = 7.12491 - 1323.06/(T - 41.23)$		Stuckey & Saylor 1940
	23.27	11 700	ebulliometry	Willingham <i>et al.</i> 1945
	14.55–80.92	$\log(p/\text{mmHg}) = 6.89324 - 1203.836/(219.924 + t)$	Antoine eq. from exptl data	
	23.271	11720	ebulliometry	Forzati <i>et al.</i> 1949
	10.98–80.95	$\log(p/\text{mmHg}) = 6.911210 - 1214.645/(221.205 + t)$	Antoine eq. from exptl data	
	25	12690	extrapolated, Antoine eq.	Dreisbach 1955
	25	12690	interpolated	Zwolinski & Wilhoit 1971
	-5.85–103.9	$\log(p/\text{mmHg}) = 6.90565 - 1211.033/(220.79 + t)$	Antoine eq.	
	-11.6 to -5.85	$\log(p/\text{mmHg}) = 9.1064 - 1885.9(t + 244.2)$	Antoine eq.	
	-58 to -30	$\log(p/\text{mmHg}) = (-0.2185 \times 10254.3/T) + 9.5560$	Antoine eq.	Weast 1972–73
	36.7 to 290.3	$\log(p/\text{mmHg}) = (-0.2185 \times 146.5/T) + 7.833714$	Antoine eq.	
	-90 to -76	$\ln(p/\text{mmHg}) = 28.0206 - 6487.2/T$	torsion effusion, regression	de Kruif & Van Ginkel 1977
	-90 to -76	$\ln(p/\text{mmHg}) = 29.535 - 5938.6/T$	weighing effusion, regr.	
	292.22 K	9585	comparative ebulliometry	Osborn & Scott 1978
	294.878 K	10 887		
	297.546 K	12 339		
	300.225 K	13 955		
	302.915 K	15 748		
	305.617 K	17 735		
	-90 to -76	$\log(p/\text{Pa}) = 14.282 - 2815/T$	torsion effusion, regression	de Kruif 1980
	-90 to -76	$\log(p/\text{Pa}) = 13.1405 - 2580/T$	weighing effusion, regr.	
	-90 to -76	$\log(p/\text{Pa}) = 13.727 - 2700/T$	effusion, mean. regression	Ambrose 1981
	23.926	8634 measured at range 16.93–108.2 °C	comparative ebulliometry	
	25.549	12430 measured at range 21.01–105 °C		
	25.534	13010 measured at range 12.8–110.3 °C		
	24.61	12470 measured at range 24.6–104.4 °C		
	20	12720	OECD methods, round robin	Schmidt-Bleek <i>et al.</i> 1982
	23	12100	gas saturation	Politcki <i>et al.</i> 1982
	313–373 K	$\ln(p/\text{MPa}) = 10.0744 - 4241.29/T$	Antoine eq.	Tsonopoulos & Wilson 1983
	280–522.6 K	$\log(p/\text{atm}) = (1 - 353.214/T) \times 10^5 (0.832\ 632 - 6.72598 \times 10^{-4} \cdot T + 6.38324 \times 10^{-7} \cdot T^2)$	Cox vapor pressure eq.	Chao <i>et al.</i> 1983
	14.5–80.9	$\log(p/\text{kPa}) = 6.01788 - 1203.677/(219.904 + t)$	Antoine eq.–Willingham data	Boublik <i>et al.</i> 1973, 1984
	21.02–105	$\log(p/\text{kPa}) = 6.01905 - 1204.637/(220.069 + t)$	Antoine eq.–Ambrose data	Boublik <i>et al.</i> 1984
	-12–3	$\log(p/\text{mmHg}) = 9.1064 - 1885.9/(244.2 + t)$	Antoine eq.–solid value	Dean 1985
	8–103	$\log(p/\text{mmHg}) = 6.90565 - 1211.033/(220.79 + t)$	Antoine eq.	Dean 1985
	25	12716	headspace GC	Hussain & Carr 1985
	-50.15–5.85	$\log(p/\text{kPa}) = 10.0091 - 2836.0/(25.31 + T)$	Antoine eq.–solid	Stephenson & Malanowski 1987
	-55.15–5.85	$\log(p/\text{kPa}) = 8.45261 - 1986.69/(-22.089 + T)$	Antoine eq.–solid	
	5.85–103.85	$\log(p/\text{kPa}) = 6.01907 - 1204.682/(-53.072 + T)$	Antoine eq.–liquid	
	79.85–104	$\log(p/\text{kPa}) = 6.06832 - 1236.034/(-48.99 + T)$	Antoine eq.–liquid	
	147–223	$\log(p/\text{kPa}) = 7.51992 - 2809.514/(-15.44 + T)$	Antoine eq.–liquid	
	-15.4	880	gas saturation	Liu & Dickhut 1994
	-5	1750		
	10	6340		
	25	13 100		
	40	26 400		
	recommended value at 25 °C: 12700±500 Pa			
Toluene	0	900	mercury manometer	Pitzer and Scott 1943
	12.5	1920		
	25	3786		
	37.5	7026		
	50	12266		
	0–50 °C	$\log(p/\text{mmHg}) = -2866.53/T - 6.7 \log T + 27.6470$	equation-manometer data	Pitzer and Scott 1943
	35.366	6360	ebulliometry	Willingham <i>et al.</i> 1945

TABLE 3. Vapor pressures and reported equations for temperature dependence of aromatic hydrocarbons—Continued

Compound	<i>t</i> /°C, <i>T</i> /K or temp range	Vapor pressure or reported equations: ( <i>P</i> <sup>°</sup> /Pa)	Method	Reference
Toluene (cont'd)	35.4–111.5	$\log(p/\text{mmHg}) = 8.953 \cdot 37 - 1343.943/(219.377 + t)$ 6400	Antoine eq-ebulliometric data ebulliometry	Forzati <i>et al.</i> 1949
	35.5	$\log(p/\text{mmHg}) = 6.955 \cdot 08 - 1345.087/(219.516 + t)$ 3792	Antoine eq-ebulliometric data extrapolated, Antoine eq.	Dreisbach 1955
	25	$\log(p/\text{mmHg}) = 6.954 \cdot 64 - 1344.000/(219.482 + t)$ 3793	Antoine eq.	Zwolinski and Wilhoit 1971
	6.36–136.4	$\log(p/\text{mmHg}) = (-0.2185 \times 9368.5/T) + 8.3300$ $\log(p/\text{mmHg}) = (-0.2185 \times 8586.0/T) + 7.719392$ 3650	Antoine eq. gas saturation-GC Cox eq.	Weast 1972–73 Politcki <i>et al.</i> 1982 Chao <i>et al.</i> 1983
	25	$\log(p/\text{atm}) = (1 - 383.737/T) \times 10^7 \cdot 0.837 \cdot 122$ $- 6.48791 \times 10^{-4} \cdot T + 5.91 \cdot 293 \times 10^{-7} \cdot T^2$ $\log(p/\text{kPa}) = 6.084 \cdot 36 - 1347.62/(219.787 + t)$ $\log(p/\text{kPa}) = 6.379 \cdot 98 - 1575.007/(249.372 + t)$ 3790	Antoine eq.-Willingham data Antoine eq.-Ambrose data headspace GC	Boublik <i>et al.</i> 1984
	35.4–111.5 °C	$\log(p/\text{kPa}) = 6.086 \cdot 27 - 1349.122/(-53.154 + T)$ $\log(p/\text{kPa}) = 6.1528 - 1376.81/(-51.1 + T)$ $\log(p/\text{kPa}) = 6.120 \cdot 72 - 1374.901/(-49.657 + T)$ $\log(p/\text{kPa}) = 6.408 \cdot 51 - 1615.834/(-15.897 + T)$ $\log(p/\text{kPa}) = 7.653 \cdot 83 - 3153.235/(188.566 + T)$ $\log(p/\text{kPa}) = 6.162 \cdot 73 - 1391.005/(-48.974 + T)$	Antoine eq. Antoine eq. Antoine eq. Antoine eq. Antoine eq.	Hussam and Carr 1985 Stephenson & Malanowski 1987
	86.86–307 °C	recommended value at 25 °C: 3800±200 Pa		
Ethylbenzene	10	387	mercury manometer	Rintelen <i>et al.</i> 1937
	30	1546		
	50	4613		
	4–75 °C	$\log(p/\text{mmHg}) = -3122.45/T - 5 \cdot \log T + 23.23680$	manometer data	Stuckey & Saylor 1940
	56.6–137	$\log(p/\text{mmHg}) = 6.94998 - 1419.315/(212.611 + t)$	Antoine eq-ebulliometric data	Willingham <i>et al.</i> 1945
	56.7–137.2	$\log(p/\text{mmHg}) = 6.95904 - 1425.464/(213.345 + t)$ 1276	Antoine eq-ebulliometric data extrapolated, Antoine eq.	Forzati <i>et al.</i> 1949 Dreisbach 1955
	25.88–163.5	$\log(p/\text{mmHg}) = 6.95719 - 1424.255/(213.206 + t)$ 1270	Antoine eq.	Zwolinski & Wilhoit 1971
	25			
	−9.8–326.5	$\log(p/\text{mmHg}) = (-0.2185 \times 9301.3/T) + 7.809470$ $\log(p/\text{atm}) = (1 - 409.229/T) \times 10^7 \cdot (0.859833$ $- 6.85948 \times 10^{-4} \cdot T + 5.94439 \times 10^{-7} \cdot T^2)$	Antoine eq. Cox eq.	Weast 1972–73 Chao <i>et al.</i> 1983
	243.2–615 K	$\log(p/\text{kPa}) = 6.08206 - 1425.305/(213.415 + t)$ $\log(p/\text{kPa}) = 6.0785 - 1421.652/(212.876 + t)$ $\ln(p/\text{MPa}) = 21.7487 - 5478.28/T - 1.53423 \cdot \ln T$ $\log(p/\text{mmHg}) = 6.95719 = -1424.255/(t + 213.21)$ $\log(p/\text{kPa}) = 6.069 \cdot 91 - 1416.922/(60.716 + T)$ $\log(p/\text{kPa}) = 6.108 \cdot 98 - 1445.262/(-57.128 + T)$ $\log(p/\text{kPa}) = 6.366 \cdot 56 - 1665.991/(-26.716 + T)$ $\log(p/\text{kPa}) = 7.491 \cdot 19 - 3056.747/(159.496 + T)$	Antoine eq.-Willingham data Antoine eq. three-term eq. Antoine eq. Antoine eq.	Boublik <i>et al.</i> 1984 Heidman <i>et al.</i> 1985 Dean 1985 Stephenson & Malanowski 1987
	25.9–92.7 °C	recommended value at 25 °C: 1270±50 Pa		
<i>o</i> -Xylene	0	215	mercury manometer	Kassel 1936
	10	477		
	20	767		
	30	1347		
	40	2280		
	50	3680		
	60	5626		
	70	8473		
	80	13186		
<i>o</i> -Xylene	0–80	$\log(p/\text{mmHg}) = -2830.0/T - 5 \cdot \log T - 23.7480$	manometer data	Kassel 1936
	10	213	mercury manometer	Rintelen <i>et al.</i> 1937
	30	987		
	50	3346		
	4–75 °C	$\log(p/\text{mmHg}) = -908.07/T - 5 \cdot \log T + 22.952 \cdot 79$	manometer data	Stuckey & Saylor 1940
	0	173	mercury manometer	Pitzer & Scott 1943
	12.5	400		
	25	800		
	37.5	1800		
	50	3400		
	60	5413		
	0–60 °C	$\log(p/\text{mmHg}) = -3327.16/T - 8.0 \cdot \log T + 31.7771$	equation-manometer data	Pitzer and Scott 1943
	63.5–145.4	$\log(p/\text{mmHg}) = 6.99937 - 1474.969/(213.714 + t)$	Antoine eq-ebulliometric data	Willingham <i>et al.</i> 1945
	64.5–145.5	$\log(p/\text{mmHg}) = 6.99891 - 1474.679/(213.686 + t)$	Antoine eq-ebulliometric data	Forzati <i>et al.</i> 1949

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TABLE 3. Vapor pressures and reported equations for temperature dependence of aromatic hydrocarbons—Continued

Compound	$t/^\circ\text{C}$ , $T/\text{K}$ or temp range	Vapor pressure or reported equations: ( $p/\text{kPa}$ )	Method	Reference
<i>o</i> -Xylene (cont'd)	25	892	extrapolated, Antoine eq.	Dreisbach 1955
	32.14–172.07	$\log(p/\text{mmHg}) = 6.99891 - 1474.679/(213.686 + t)$	Antoine eq.	Zwolinski & Wilhoit 1971
	25	880		
	–3.8–144.4	$\log(p/\text{mmHg}) = (-0.2185 \times 9998.5/T) + 8.147551$	Antoine eq.	Weast 1972–73
	253–631.6 K	$\log(p/\text{atm}) = (1 - 417.496/T) \times 10^{-7} (0.855257 - 6.48662 \times 10^{-4} \cdot T + 5.53883 \times 10^{-7} \cdot T^2)$	Cox eq.	Chao <i>et al.</i> 1983
	0–50 °C	$\log(p/\text{kPa}) = 5.9422 - 1387.336/(206.409 + t)$	Antoine eq.-Pitzer data	Boublik <i>et al.</i> 1984
	63–145 °C	$\log(p/\text{kPa}) = 6.12699 - 1476.753/(213.977 + t)$	Antoine eq.-Willingham data	
	32–172	$\log(p/\text{mmHg}) = 6.99891 - 1474.679/(t + 213.69)$	Antoine eq.	Dean 1985
	333–419 K	$\log(p/\text{kPa}) = 6.13132 - 1480.155/(-58.804 + T)$	Antoine eq.	Stephenson & Malanowski 1987
	416–473 K	$\log(p/\text{kPa}) = 6.15921 - 1502.949/(-55.725 + T)$		
	471–571 K	$\log(p/\text{kPa}) = 6.46119 - 1772.963/(-18.84 + T)$		
	567–630 K	$\log(p/\text{kPa}) = 7.91427 - 3735.582/(229.953 + T)$		
	recommended value at 25 °C: 880±40 Pa			
<i>m</i> -Xylene	0	228	mercury manometer	Kassel 1936
	10	433		
	20	833		
	30	1480		
	40	2533		
	50	4173		
	60	6626		
	70	10212		
	80	15280		
	0–80	$\log(p/\text{mmHg}) = -2876.3/T - 5 \cdot \log T + 22.9425$	manometer data	Kassel 1936
	10	293	mercury manometer	Rintelen <i>et al.</i> 1937
	30	1213		
	50	3906		
	4–75 °C	$\log(p/\text{mmHg}) = -2870.38/T - 5 \cdot \log T + 22.92341$	manometer data	Stuckey & Saylor 1940
	0	233	mercury manometer	Pitzer & Scott 1943
	12.5	520		
	25	1113		
	37.7	2220		
	50	4160		
	60	6600		
	0–60 °C	$\log(p/\text{mmHg}) = -2871.66/T - 5.0 \cdot \log T + 22.9270$	equation-manometer data	Pitzer and Scott 1943
	59.2–140	$\log(p/\text{mmHg}) = 7.00343 - 1458.214/(214.609 + t)$	Antoine eq.-ebulliometric data	Willingham <i>et al.</i> 1945
	59.3–140.1	$\log(p/\text{mmHg}) = 7.00849 - 1461.925/(215.073 + t)$	Antoine eq.-ebulliometric data	Forzati <i>et al.</i> 1949
	23	1113	extrapolated, Antoine eq.	Dreisbach 1955
	28.24–166.39	$\log(p/\text{mmHg}) = 7.00908 - 1462.266/(215.105 + t)$	Antoine eq.	Zwolinski & Wilhoit 1971
	25	1107	extrapolated-Antoine eq.	
	–6.9–139.1	$\log(p/\text{mmHg}) = (-0.2185 \times 9904.2/T) + 8.167049$	Antoine eq.	Weast 1972–73
	243–619.2 K	$\log(p/\text{atm}) = (1 - 412.135/T) \times 10^{-7} (0.858941 - 6.73249 \times 10^{-4} \cdot T + 5.87430 \times 10^{-7} \cdot T^2)$	Cox eq.	Chao <i>et al.</i> 1983
	0–60 °C	$\log(p/\text{kPa}) = 6.4729 - 1641.628/(230.899 + t)$	Antoine eq.-Pitzer data	Boublik <i>et al.</i> 1984
	59–140 °C	$\log(p/\text{kPa}) = 6.13232 - 1460.805 + t$	Antoine eq.-Willingham data	
	28–166 K	$\log(p/\text{mmHg}) = 7.00908 - 1462.266/(t + 215.11)$	Antoine eq.	Dean 1985
	331–415 K	$\log(p/\text{kPa}) = 6.14083 - 1467.244/(57.442 + T)$	Antoine eq.	Stephenson & Malanowski 1987
	267–301 K	$\log(p/\text{kPa}) = 5.76037 - 1292.224/(-72.052 + T)$		
	412–462 K	$\log(p/\text{kPa}) = 6.17035 - 1490.184/(-24.592 + T)$		
	461–534 K	$\log(p/\text{kPa}) = 6.42535 - 1710.901/(-24.591 + T)$		
	550–617 K	$\log(p/\text{kPa}) = 7.59221 - 3163.74/(165.278 + T)$		
	recommended value at 25 °C: 1100±100 Pa			
<i>p</i> -Xylene	0	208	mercury manometer	Kassel 1936
	10	415		
	20	787		
	30	1427		
	40	2453		
	50	4093		
	60	6573		
	70	10226		
	80	15452		
	0–80	$\log(p/\text{mmHg}) = -2930.0/T - 5 \cdot \log T + 23.1000$	manometer data	Kassel 1936

TABLE 3. Vapor pressures and reported equations for temperature dependence of aromatic hydrocarbons—Continued

Compound	$t/^\circ\text{C}$ , $T/\text{K}$ or temp range	Vapor pressure or reported equations: ( $\text{p}^5/\text{Pa}$ )	Method	Reference
<i>p</i> -Xylene (cont'd)	10	306.6	mercury manometer	Rintelen <i>et al.</i> 1937
	30	1427		
	50	4306		
	13–75 °C	$\log(p/\text{mmHg}) = -2851.90/T - 5 \cdot \log T + 22.88436$	manometer data	Stuckey & Saylor 1940
	0	180	mercury manometer, solid	Pitzer & Scott 1943
	12.5	540	mercury manometer, solid	
	25	1187	mercury manometer, liquid	
	37.5	2333		
	50	4346		
	60	6846		
	0–13.23 °C	$\log(p/\text{mmHg}) = -3141.33/T + 11.6092$	eq.-manometer data, solid	Pitzer and Scott 1943
	13.23–60 °C	$\log(p/\text{mmHg}) = -3080.31/T - 6.7 \cdot \log T + 27.8581$	eq.-manometer data, liquid	
	58.3–139.8	$\log(p/\text{mmHg}) = 6.98648 - 1450.688/(214.990+t)$	Antoine eq.-ebulliometric data	Willingham <i>et al.</i> 1945
	58.4–139.3	$\log(p/\text{mmHg}) = 6.99184 - 1454.328/(215.411+t)$	Antoine eq.-ebulliometric data	Forzati <i>et al.</i> 1949
	25	1175	extrapolated, Antoine eq.	Dreisbach 1955
	27.32–165.73	$\log(p/\text{mmHg}) = 6.99052 - 1453.430/(215.307+t)$	Antoine eq.	Zwolinski and Wilhoit 1971
	25	1173	extrapolated-Antoine eq.	
	−8.1–138.3	$\log(p/\text{mmHg}) = (-0.2185 \times 9809.9/T) + 8.124805$	Antoine eq.	Weast 1972–73
	−26.043	11.60	inclined-piston manometry	Osborn and Douslin 1975
	−21.164	19.598		
	−16.277	33.197		
	−10.403	60.794		
	−4.995	103.856		
	−0.006	170.52		
	4.912	272.37		
	9.838	429.16		
	12.483	544.35		
	247 K to t.p.	$\log p/p_\Phi = A(1-\Phi/T); \Phi = 286.374 \text{ K}, p_\Phi = 4.354,$ and $A = -0.303858 + 9.78538 \times 10^{-3} \cdot T - 1.77986 \times 10^{-5} \cdot T^2$	solid, Cox eq.	Osborn and Douslin 1974
	13.285	581.68	inclined-piston manometry	Osborn and Douslin 1974
	15.004	648.87		
	17.474	755.39		
	20.015	880.31		
	67.795	9590	comparative ebulliometry	Osborn and Douslin 1974
	70.881	10892		
	73.978	12344		
	77.086	13960		
	80.206	15752		
	83.339	17737		
	86.483	19933		
	92.084	25023		
	t.p. to 453 K	$\log p/p_\Phi = A(1-\Phi/T); \Phi = 286.354 \text{ K}, p_\Phi = 4.354,$ and $\log A = 1.004831 - 5.00738 \times 10^{-4} \cdot T + 4.06552 \times 10^{-7} \cdot T^2$	liquid, Cox equation	Osborn & Douslin 1974
	290–618 K	$\log(p/\text{atm}) = (1 - 411.503/T) \times 10^{-5} (0.847730 - 6.49489 \times 10^{-4} \cdot T + 5.59094 \times 10^{-7} \cdot T^2)$	Cox eq.	Chao <i>et al.</i> 1983
	58.3–139 °C	$\log(p/\text{kPa}) = 6.11376 - 1452.215/(215.518+t)$	Antoine eq.-Willingham data	Boublik <i>et al.</i> 1984
	99–179 °C	$\log(p/\text{kPa}) = 6.11513 - 1453.812/(215.242+t)$	Antoine eq.-Osborn data	
	27–166	$\log(p/\text{mmHg}) = 6.99052 - 1453.430/(t+215.31)$	Antoine eq.	Dean 1985
	247–286 K	$\log(p/\text{kPa}) = 15.50091 - 6327.014/(115.724+t)$	Antoine eq., solid	Stephenson & Malanowski 1987
	286–453 K	$\log(p/\text{kPa}) = 6.14779 - 1475.767/( -55.241+t)$	Antoine eq., liquid	Stephenson & Malanowski 1987
	411–463 K	$\log(p/\text{kPa}) = 6.14049 - 1472.733/( -55.342+t)$	Stephenson & Malanowski 1987	
	460–553 K	$\log(p/\text{kPa}) = 6.44333 - 1735.196/( -19.846+t)$	Stephenson & Malanowski 1987	
	551–616 K	$\log(p/\text{kPa}) = 7.84182 - 3543.356/(208.522+t)$	Stephenson & Malanowski 1987	
	recommended value at 25 °C: 1170±10 Pa			
1,2,3-Trimethylbenzene	90.3–177.7	$\log(p/\text{mmHg}) = 7.04082 - 1593.958/(207.078+t)$	Antoine eq.-ebulliometric data	Forzati <i>et al.</i> 1949
	25	206	extrapolated, Antoine eq.	Dreisbach 1955
	56.79–205.36	$\log(p/\text{mmHg}) = 7.04082 - 1593.958/(207.078+t)$	Antoine eq.	Zwolinski & Wilhoit 1971
	16.8–176.1	$\log(p/\text{mmHg}) = (-0.2185 \times 10781.9/T) + 8.154069$	Antoine eq.	Weast 1972–73
	290–660 K	$\log(p/\text{atm}) = (1 - 449.175/T) \times 10^{-5} (0.869047 - 6.33423 \times 10^{-4} \cdot T + 5.14963 \times 10^{-7} \cdot T^2)$	Cox eq.	Chao <i>et al.</i> 1983
	25			
	90.33–177	$\log(p/\text{kPa}) = 6.16365 - 1592.422/(206.905+t)$	Forzati <i>et al.</i> 1949 data	Boublik <i>et al.</i> 1984
	57–205	$\log(p/\text{mmHg}) = 7.04082 - 1593.958/(t+207.08)$	Antoine eq.	Dean 1985
	363–456 K	$\log(p/\text{kPa}) = 6.16447 - 1593.776/( -66.032+t)$	Antoine eq.	Stephenson & Malanowski 1987

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TABLE 3. Vapor pressures and reported equations for temperature dependence of aromatic hydrocarbons—Continued

Compound	<i>t/°C, T/K or temp range</i>	Vapor pressure or reported equations: ( $p^S/\text{Pa}$ )	Method	Reference
recommended value at 25 °C: 200 Pa				
1,2,4-Trimethylbenzene	84.8–170.4	$\log(p/\text{mmHg}) = 7.03483 - 1573.207/(208.564 + t)$	Antoine eq-ebulliometric data	Forziati <i>et al.</i> 1949
	25	280	extrapolated, Antoine eq.	Dreisbach 1955
	51.75–198.2	$\log(p/\text{mmHg}) = 7.04383 - 1573.267/(208.564 + t)$	Antoine eq.	Zwolinski & Wilhoit 1971
	13.6–169.2	$\log(p/\text{mmHg}) = (-0.2185 \times 10710.27) + 8.209013$	Antoine eq.	Weast 1972–73
	253–645 K	$\log(p/\text{atm}) = (1 - 443.537/T) \times 10^7 (0.848724 - 5.41424 \times 10^{-4} \cdot T + 4.22211 \times 10^{-7} \cdot T^2)$	Cox eq.	Chao <i>et al.</i> 1983
	84.8–170.4	$\log(p/\text{kPa}) = 6.16282 - 1569.06/(208.089 + t)$	Forziati <i>et al.</i> 1949 data	Boublik <i>et al.</i> 1984
	52–198	$\log(p/\text{mmHg}) = 7.04383 - 1573.267/(t + 208.56)$	Antoine eq.	Dean 1985
	357–450 K	$\log(p/\text{kPa}) = 6.16695 - 1572.687/( - 64.593 + T)$	Antoine eq.	Stephenson & Malanowski 1987
recommended value at 25 °C: 270 ± 20 Pa				
1,3,5-Trimethylbenzene	0	58.7	mercury manometer	Kassel 1936
	10	124		
	20	248		
	30	521		
	40	844		
	50	1467		
	60	2440		
	70	3933		
	80	6133		
	0–100	$\log(p/\text{mmHg}) = -3104.5/T - 5 \cdot \log T + 23.1929$	manometer data	Kassel 1936
	10	80.0	mercury manometer	Rintelen <i>et al.</i> 1937
	30	507		
	50	1533		
	4–75 °C	$\log(p/\text{mmHg}) = -3122.45/T - 5 \cdot \log T + 23.23680$	manometer data	Stuckey & Saylor 1940
	81.5–164.7	$\log(p/\text{mmHg}) = 7.07437 - 1569.622/(209.578 + t)$	Antoine eq-ebulliometric data	Forziati <i>et al.</i> 1949
	25	331	extrapolated, Antoine eq.	Dreisbach 1955
	48.82–193.07	$\log(p/\text{mmHg}) = 7.07436 - 1569.622/(209.578 + t)$	Antoine eq.	Zwolinski & Wilhoit 1971
	9.6–164.7	$\log(p/\text{mmHg}) = (-0.2185 \times 10516.8/T) + 8.161663$	Antoine eq.	Weast 1972–73
	253–635 K	$\log(p/\text{atm}) = (1 - 437.769/T) \times 10^7 (0.87945 - 6.55508 \times 10^{-4} \cdot T + 5.47586 \times 10^{-7} \cdot T^2)$	Cox eq.	Chao <i>et al.</i> 1983
	81.5–165.7	$\log(p/\text{kPa}) = 6.20212 - 1571.575/(209.79 + t)$	Forziati <i>et al.</i> 1949 data	Boublik <i>et al.</i> 1984
	49–193	$\log(p/\text{mmHg}) = 7.07436 - 1569.622/(t + 209.58)$	Antoine eq.	Dean 1985
	354–445 K	$\log(p/\text{kPa}) = 6.19762 - 1569.149/(-63.565 + T)$	Antoine eq.	Stephenson & Malanowski 1987
	249–356 K	$\log(p/\text{kPa}) = 6.62312 - 1810.653/(-43.307 + T)$	Antoine eq.	Stephenson & Malanowski 1987
recommended value at 25 °C: 325 ± 20 Pa				
<i>o</i> -Ethyl toluene	81.1–166.2	$\log(p/\text{mmHg}) = 7.00314 - 1535.374/(207.300 + t)$	Antoine eq-ebulliometric data	Forziati <i>et al.</i> 1949
	25	336	extrapolated, Antoine eq.	Dreisbach 1955
	48.46–193.9	$\log(p/\text{mmHg}) = 7.00314 - 1535.374/(207.300 + t)$	Antoine eq.	Zwolinski & Wilhoit 1971
	9.4–165.1	$\log(p/\text{mmHg}) = (-0.2185 \times 10488.8/T) + 8.141032$	Antoine eq.	Weast 1972–73
	285–645 K	$\log(p/\text{atm}) = (1 - 438.357/T) \times 10^7 (0.863837 - 6.34917 \times 10^{-4} \cdot T + 5.19164 \times 10^{-7} \cdot T^2)$	Cox eq.	Chao <i>et al.</i> 1983
	81–166	$\log(p/\text{kPa}) = 6.11997 - 1529.684/(206.548 + t)$	Antoine eq-Forziati data	Boublik <i>et al.</i> 1984
	353–443 K	$\log(p/\text{kPa}) = 6.1229 - 1532.449/(-66.123 + T)$	Antoine eq., liquid	Stephenson & Malanowski 1987
recommended value at 25 °C: 330 Pa				
<i>m</i> -Ethyl toluene	78.1–162.3	$\log(p/\text{mmHg}) = 7.01582 - 1529.184/(206.509 + t)$	Antoine eq-ebulliometric data	Forziati <i>et al.</i> 1949
	25	399	extrapolated, Antoine eq.	Dreisbach 1955
	45.68–189.7	$\log(p/\text{mmHg}) = 7.01582 - 1529.184/(208.509 + t)$	Antoine eq.	Zwolinski & Wilhoit 1971
	7.4–161.3	$\log(p/\text{mmHg}) = (-0.2185 \times 10416.6/T) + 8.152199$	Antoine eq.	Weast 1972–73
	280–635 K	$\log(p/\text{atm}) = (1 - 434.538/T) \times 10^7 (0.861499 - 6.30303 \times 10^{-4} \cdot T + 5.19848 \times 10^{-7} \cdot T^2)$	Cox eq.	Chao <i>et al.</i> 1983
	78–165 °C	$\log(p/\text{kPa}) = 6.12947 - 1531.584/(161.989 + t)$	Antoine eq-Forziati data	Boublik <i>et al.</i> 1984
	348–438 K	$\log(p/\text{kPa}) = 6.13801 - 1527.983/(-64.715 + T)$	Antoine eq., liquid	Stephenson & Malanowski 1987
recommended value at 25 °C: 399 Pa				
<i>p</i> -Ethyl toluene	78.3–163.0	$\log(p/\text{mmHg}) = 6.99801 - 1527.113/(208.921 + t)$	Antoine eq-ebulliometric data	Forziati <i>et al.</i> 1949
	25	402	extrapolated, Antoine eq.	Dreisbach 1955
	45.68–190.64	$\log(p/\text{mmHg}) = 6.99802 - 1527.113/(208.921 + t)$	Antoine eq.	Zwolinski & Wilhoit 1971
	7.7–162	$\log(p/\text{mmHg}) = (-0.2185 \times 10461.1/T) + 8.175267$	Antoine eq.	Weast 1972–73
	280–635 K	$\log(p/\text{atm}) = (1 - 435.228/T) \times 10^7 (0.856105 - 6.18307 \times 10^{-4} \cdot T + 5.08568 \times 10^{-7} \cdot T^2)$	Cox eq.	Chao <i>et al.</i> 1983





TABLE 3. Vapor pressures and reported equations for temperature dependence of aromatic hydrocarbons—Continued

Compound	t/°C, T/K or temp range	Vapor pressure or reported equations: (p <sup>s</sup> /Pa)	Method	Reference
1,3-Diethylbenzene (cont'd)	21.7–182.2	$\log(p/\text{mmHg}) = (-0.2185 \times 109.93) \frac{9.9}{T} + 8.177452$	Antoine eq.	Weast 1972–73
	295–650 K	$\log(p/\text{atm}) = (1 - 454.3627/T) \times 10^{-6} (0.889714 - 6.94128 \times 10^{-4} \cdot T + 5.62739 \times 10^{-7} \cdot T^2)$	Cox eq.	Chao <i>et al.</i> 1983
	368–457 K	$\log(p/\text{kPa}) = 6.12631 - 1573.709/( -72.314 + T)$	Antoine eq., liquid	Stephenson & Malanowski 1987
1,4-Diethylbenzene	recommended value at 25 °C: 151 Pa			
	96.8–184.8	$\log(p/\text{mmHg}) = 7.00054 - 1589.272/(202.019 + t)$	Antoine eq.—ebulliometric extrapolated, Antoine eq.	Forzati <i>et al.</i> 1949
n-Pentylbenzene	25	140.5	Antoine eq.	Dreisbach 1955
	62.83–213.59	$\log(p/\text{mmHg}) = 6.99820 - 1588.31/(201.970 + t)$	Zwolinski & Wilhoit 1971	
	19.4–182.5	$\log(p/\text{mmHg}) = (-0.2185 \times 10746.3/T) + 8.057804$	Antoine eq.	Weast 1972–73
	295–655 K	$\log(p/\text{atm}) = (1 - 456.809/T) \times 10^{-6} (0.893772 - 7.13376 \times 10^{-4} \cdot T + 5.76066 \times 10^{-7} \cdot T^2)$	Cox eq.	Chao <i>et al.</i> 1983
	369–464 K	$\log(p/\text{kPa}) = 6.12548 - 1589.933/( -70.995 + T)$	Antoine eq., liquid	Stephenson & Malanowski 1987
Pentamethylbenzene	recommended value at 25 °C: 140.5 Pa			
	25	43.73	extrapolated, Antoine eq.	Dreisbach 1955
n-Hexylbenzene	80–237	$\log(p/\text{mmHg}) = 6.97833 - 1639.91/(194.76 + t)$	Antoine eq.	Zwolinski & Wilhoit 1971
	recommended value at 25 °C: 44.0 Pa			
Hexamethylbenzene	338–503 K	$\log(p/\text{kPa}) = 6.3509 - 1867/( -75.15 + T)$	Antoine eq., liquid	Stephenson & Malanowski 1987
	recommended value at 25 °C: 9.52 Pa			
n-Heptylbenzene	96–258	$\log(p/\text{mmHg}) = 6.9853 - 1700.5/(188.2 + t)$	Antoine eq.	Zwolinski & Wilhoit 1971
	recommended value at 25 °C: 13.6 Pa			
n-Octylbenzene	314–363 K	$R \cdot \ln(p/\text{atm}) = \Delta H_o/T + [0.136595 \cdot T - 2.724 \times 10^{-4} \cdot T^2 + 2.008379 \times 10^{-7} \cdot T^3] + I$ $\Delta H_o = 17355 \text{ kcal mol}^{-1}, I = 5.1029 \text{ cal K}^{-1}\text{mol}^{-1}$	Overberger <i>et al.</i> 1969	
	29.95	$\log(p/\text{mmHg}) = 13.134 - 3855/(T - 21)$	Antoine eq.	Ambrose <i>et al.</i> 1976
	35.07	0.28 measured range 303–343 K	static-diaphragm gauge	Ambrose <i>et al.</i> 1976
	40.02	0.49		
	44.96	0.85		
	49.95	1.41		
	50.04	2.34		
	59.95	3.81		
	65.45	6.05		
	69.87	9.39		
	25	14.4		
	303–343 K	0.16 303–343 K	calcd from vap. pres. eq.	
	303–343 K	$\log(p/\text{Pa}) = 13.134 - 3855/(T - 21.0)$	Antoine eq. from exptl. data	Ambrose <i>et al.</i> 1976
Decylbenzene	443–537 K	$\log(p/\text{atm}) = (1 - 571.163/T) \times 10^{-6} (1.00973 - 5.04725 \times 10^{-4} \cdot T - 6.30130 \times 10^{-7} \cdot T^2)$	Cox eq.	Chao <i>et al.</i> 1983
	recommended value at 25 °C: 0.155 Pa			
	112–279	$\log(p/\text{mmHg}) = 7.0006 - 1761.2/(181.5 + t)$	Antoine eq.	Zwolinski & Wilhoit 1971
Styrene	66.2–233	$\log(p/\text{mmHg}) = (-0.2185 \times 13535.4/T) + 8.732602$	Antoine eq.	Weast 1972–73
	127–298	$\log(p/\text{mmHg}) = 7.0086 - 1812.2/(174.6 + t)$	Antoine eq.	Zwolinski & Wilhoit 1971
Decylbenzene	recommended value at 25 °C:			
	203–298	$\log(p/\text{mmHg}) = 7.03596 - 1903.96/(t + 160.33)$	Antoine eq.	Dean 1985
	202.9–297.9	$\log(p/\text{mmHg}) = 7.03462 - 1904.132/(160.318 + t)$	Antoine eq. from exptl. data	Camin <i>et al.</i> 1954
	29.92	1093		Dreyer <i>et al.</i> 1955
	39.21	1827		
	60.04	5106		
	74.42	9639		
	85.53	14999		
	99.51	25105		
	110.06	35877		
	80 °C–120 °C	$\log(p/\text{mmHg}) = -3151/T - 6.294 \cdot \log T + 26.92$	extrapolated, Antoine eq.	Buck <i>et al.</i> 1949
	25	807		Dreisbach 1955
	32.4	1333		Chaiyavech & van Winkle 1959
	45.6	2666		
	53.86	4000		
	60.05	5333		
	65.45	6666		
	76.6	10666		

TABLE 3. Vapor pressures and reported equations for temperature dependence of aromatic hydrocarbons—Continued

Compound	t/°C, T/K or temp range	Vapor pressure or reported equations: (p³/Pa)	Method	Reference
Styrene (cont'd)	82.19	13332		
	below 60 °C	$\log(p/\text{mmHg}) = 8.26960 - 2221.3/T$	Antoine eq.	Chaiyavech & van Winkle 1959
	-7–145.2	$\log(p/\text{mmHg}) = (-0.2185 \times 9634.7/T) + 7.922049$	Antoine eq.	Weast 1972–73
	29.9–144.8	$\log(p/\text{Torr}) = 7.06623 - 1507.434/(t + 214.985)$	Antoine eq., Dreyer data	Boublik <i>et al.</i> 1973
	32.4–62.19	$\log(p/\text{Torr}) = 7.14016 - 1574.511/(t + 224.087)$	Antoine eq., Chaiyavech data	Boublik <i>et al.</i> 1973
	281–528 K	$\log(p/\text{atm}) = (1 - 418.675/T) \times 10^{-6} (0.886470 - 8.14267 \times 10^{-4} \cdot T + 7.57896 \times 10^{-7} \cdot T^2)$	Cox eq.	Chao <i>et al.</i> 1983
	29.9–144.8	$\log(p/\text{kPa}) = 6.235 - 1557.406/(t + 222.538)$	Antoine eq., Chaiyavech data	Boublik <i>et al.</i> 1984
	32.4–62.19	$\log(p/\text{kPa}) = 6.18301 - 1502.162/(t + 214.42)$	Antoine eq., Dreyer data	
	32–82	$\log(p/\text{mmHg}) = 7.14016 - 1574/(t + 224.09)$	Antoine eq.	Dean 1985
	245–334 K	$\log(p/\text{kPa}) = 7.3945 - 2221.3/T$	Antoine eq.	Stephenson & Malanowski 1987
	334–419 K	$\log(p/\text{kPa}) = 6.08201 - 1445.58/(-63.72 + T)$	Antoine eq.	
	recommended value at 25 °C: 880±40 Pa			
<i>o</i> -methylstyrene	32.01	387		Clements <i>et al.</i> 1953
	40.85	663		
	58.51	1753		
	72.2	3113		
	82.8	5529		
	100.35	11310		
	25	240.8	extrapolated, Antoine eq.	Dreisbach 1955
	32–12.4	$\log(p/\text{Torr}) = 7.21287 - 1644.083/(t + 214.585)$	Antoine eq.	Boublik <i>et al.</i> 1973
	303–385.5 K	$\log(p/\text{atm}) = (1 - 443.504/T) \times 10^{-6} (0.890379 - 7.17666 \times 10^{-4} \cdot T + 5.97058 \times 10^{-7} \cdot T^2)$	Cox eq.	Chao <i>et al.</i> 1983
	32–112.4	$\log(p/\text{kPa}) = 6.33107 - 1564.74/(t + 214.219)$	Antoine eq.	Boublik <i>et al.</i> 1984
	32–112	$\log(p/\text{mmHg}) = 7.2129 - 1644.08/(t + 214.59)$	Antoine eq.	Dean 1985
	75–255	$\log(p/\text{mmHg}) = 6.884611 - 1485.4/(t + 200.0)$		
	305–385 K	$\log(p/\text{kPa}) = 6.27762 - 1628.405/(-71.183 + T)$	Antoine eq.	Stephenson & Malanowski 1987
	recommended value at 25 °C: 240.8 Pa			
<i>m</i> -Methylstyrene	80–120	$\log(p/\text{mmHg}) = -3463/T - 7.533 \cdot \log T + 30.9$	Antoine eq. from exptl. data	Buck <i>et al.</i> 1949
	25	257	extrapolated, Antoine eq.	Dreisbach 1955
	67.6–169	$\log(p/\text{Torr}) = 7.06423 - 1563.74/(t + 204.083)$	Antoine eq.	Boublik <i>et al.</i> 1973
	41.7–112	$\log(p/\text{Torr}) = 7.11224 - 1516.091/(t + 210.809)$	Antoine eq.	
	315–442 K	$\log(p/\text{atm}) = (1 - 442.985/T) \times 10^{-6} (0.885861 - 7.19653 \times 10^{-4} \cdot T + 6.75359 \times 10^{-7} \cdot T^2)$	Cox eq.	Chao <i>et al.</i> 1983
	67.6–169	$\log(p/\text{kPa}) = 6.17253 - 1553.744/(t + 202.922)$	Antoine eq.	Boublik <i>et al.</i> 1984
	41.7–112	$\log(p/\text{kPa}) = 6.22823 - 1535.073/(t + 200.732)$	Antoine eq.	
	10–72	$\log(p/\text{mmHg}) = 7.25734 - 1695.4/(t + 220.0)$	Antoine eq.	Dean 1985
	72–250	$\log(p/\text{mmHg}) = 6.98728 - 1471.44/(t + 200.0)$		
	314–385 K	$\log(p/\text{kPa}) = 6.07569 - 1520.412/(-71.183 + T)$	Antoine eq.	Stephenson & Malanowski 1987
	recommended value at 25 °C: 257 Pa			
<i>p</i> -Methylstyrene	80–120	$\log(p/\text{mmHg}) = -3476/T - 6.923 \cdot \log T + 29.03$	Antoine eq. from exptl. data	Buck <i>et al.</i> 1949
	31.82	376		Clements <i>et al.</i> 1953
	41.76	689		
	52.17	1207		
	66.62	1538		
	75.4	3858		
	82.44	5206		
	25	241.5	extrapolated, Antoine eq.	Dreisbach 1955
	68.6–170	$\log(p/\text{Torr}) = 7.01119 - 1353.073/(t + 200.732)$	Antoine eq.	Boublik <i>et al.</i> 1973
	31.8–97	$\log(p/\text{kPa}) = 7.04425 - 1591.082/(t + 209.441)$	Antoine eq., Clements data	
	289–443 K	$\log(p/\text{atm}) = (1 - 443.748/T) \times 10^{-6} (0.875061 - 7.08160 \times 10^{-4} \cdot T + 7.33461 \times 10^{-7} \cdot T^2)$	Cox eq.	Chao <i>et al.</i> 1983
	68.6–170	$\log(p/\text{kPa}) = 6.11531 - 1521.514/(t + 199.299)$	Antoine eq.	Boublik <i>et al.</i> 1984
	31.8–97	$\log(p/\text{kPa}) = 6.16144 - 1586.596/(t + 209.046)$	Antoine eq.	
	68–170	$\log(p/\text{mmHg}) = 7.0112 - 1535.1/(t + 200.7)$	Antoine eq.	Dean 1985
	304–370 K	$\log(p/\text{kPa}) = 6.1732 - 1594.747/(-63.261 + T)$	Antoine eq.	Stephenson & Malanowski 1987
	recommended value at 25 °C: 2412 Pa			
$\alpha$ -Methylstyrene	25	333	extrapolated, Antoine eq.	Dreisbach 1955
	7.4–165.4	$\log(p/\text{mmHg}) = (-0.2185 \times 10214.6/T) + 7.959753$	Antoine eq.	Weast 1972–73
	not specify	$\log(p/\text{mmHg}) = 6.92366 - 1486.88/(t + 202.4)$	Antoine eq.	Dean 1985
	343–493 K	$\log(p/\text{kPa}) = 6.04856 - 1486.88/(-70.75 + T)$	Antoine eq.	Stephenson & Malanowski 1987
	353–413 K	$\log(p/\text{kPa}) = 6.294 - 1599.88/(-63.72 + T)$	Antoine eq.	Stephenson & Malanowski 1987
	recommended value at 25 °C: 333 Pa			

TABLE 3. Vapor pressures and reported equations for temperature dependence of aromatic hydrocarbons—Continued

Compound	$t/^\circ\text{C}$ , $T/\text{K}$ or temp range	Vapor pressure or reported equations: ( $\text{Pa}^3/\text{Pa}$ )	Method	Reference
$\beta$ -Methylstyrene	25	267	extrapolated, Antoine eq.	Dreisbach 1955
	17.5–179	$\log(p/\text{mmHg}) = (-0.2185 \times 10701.3/T) + 8.071487$ $\log(p/\text{mmHg}) = 6.92339 - 1469.80(t+201.0)$	Antoine eq.	Weast 1972–73
	348–498 K	$\log(p/\text{kPa}) = 6.04829 - 1499.8(-72.15+T)$	Antoine eq., <i>cis</i> -Antoine eq., <i>trans</i> -	Stephenson & Malanowski 1987
	291–452 K	$\log(p/\text{kPa}) = 6.58873 - 1915.94(-33.996+T)$		Stephenson & Malanowski 1987
Indan	355–482.3 K	$\log(p/\text{kPa}) = 6.10462 - 1574.16(T - 67.079)$	comparative ebulliometry	Ambrose & Sprake 1976
	25	204	extrapolated, expd. data	Ambrose & Sprake 1976
	374.3–465.6 K	9585–143240	ebulliometry	Osborn & Scott 1978
	81.86–209.3	$\log(p/\text{kPa}) = 6.1012 - 1571.723/(205.798+t)$	Antoine eq.	Boublik <i>et al.</i> 1984
	372–466 K	$\log(p/\text{Pa}) = 6.11622 - 1580.375/(-66.49+T)$	Antoine eq.	Stephenson & Malanowski 1987
Naphthalene	recommended value at 25 °C: 230 Pa			
	87–224	$\log(p/\text{mmHg}) = 7.901 - 2465/T$	static isoteniscope method	Mortimer & Murphy 1923
	10	2.32	effusion, solid	Swan & Mack 1925
	20	8.64		
	30	23.60		
	10–30	$\log(p/\text{mmHg}) = -29.820/T - 200.682 \cdot \log T + 595.642$		
	15–33	$\log(p/\text{mmHg}) = 10.40 - 3429/T$	effusion	Zil'berman-Granovskaya 1940
	25	14.26	interpolated, manometric data	Sears & Hopke 1949
	10	2.053		
	20	8.533		
	30	21.865		
	19–35	$\log(p/\text{mmHg}) = -108.3/(t+27) + 1.115$	pressure gauge data	Sears & Hopke 1949
	19–35	$\log(p/\text{Pa}) = 12.61 - 3422/T$	regression*	from Sears & Hopke 1949
	25	10.8	extrapolated, effusion data	Bradley & Cleasby 1953
	6.7	1.627	effusion	
	8.1	1.88		
	12.3	2.96		
	12.7	3.133		
	13.85	3.506		
	15.65	4.266		
	16.85	4.666		
	17.35	5.093		
	17.55	5.106		
	18.7	5.84		
	20.7	7.119		
	6.7–20.7	$\log(p/\text{mmHg}) = -3783/T + 10.597$	regression, expd. data	Bradley & Cleasby 1953
126.3–218.6	126.3–218.6	$\log(p/\text{mmHg}) = 6.84577 - 1606.529/(187.227+t)$	Antoine eq.-expd. data	Camin & Rossini 1955
	–20–10	$\log(p/\text{mmHg}) = 10.75 - 3616/T$	effusion, solid	Hoyer & Peperle 1958
	25	10.98 measured temp range 40–80 °C	Hg manometer, extrapolated	Fowler <i>et al.</i> 1968
		$\log(p/\text{mmHg}) = 9.58102 - 2619.91/(t+220.651)$	Antoine eq. 40–80 °C	Fowler <i>et al.</i> 1968
		$\log(p/\text{mmHg}) = 7.03382 - 1756.91/(t+204.937)$	Antoine eq. 81–180 °C	Fowler <i>et al.</i> 1968
	25	30.66	extrapolated-Antoine eq.	Zwolinski & Wilhoit 1971
		$\log(p/\text{mmHg}) = 7.01065 - 1733.71/(201.859+t)$	Antoine eq.	
	0–80	$\log(p/\text{mmHg}) = (-0.2185 \times 17065.2/T) + 11.4500$	Antoine eq.	Weast 1972–73
	52.6–217.9	$\log(p/\text{mmHg}) = (-0.2185 \times 12311.6/T) + 8.413089$	Antoine eq.	
	25	6.56	evaporation rate	Gückel <i>et al.</i> 1973
	25	10.9	gas saturation	Sinke 1974
	–43.15	0.000283		
	–33.15	0.00837		
	–13.15	0.1443		
	6.85	1.6305		
	25	10.932		
	26.85	13.092		
	46.85	79.727		
	66.85	386.5		
	80.28	999.8		
	–53 to 80	$\log(p/\text{Pa}) = 13.83 - 3817/T$	gas sat., regression*	Sinke 1974
	9.0	2.537	Knudsen effusion method	Radchenko & Kitaigorodskii 74
	10.7	3.113		
	12.5	5.637		
	14.4	7.546		
	16.3	19.585		
	18.2	30.96		
	20.0	48.36		
	21.95	74.19		
	23.91	112.55		

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TABLE 3. Vapor pressures and reported equations for temperature dependence of aromatic hydrocarbons—Continued

Compound	$t/^\circ\text{C}$ , $T/\text{K}$ or temp range	Vapor pressure or reported equations: ( $p^2/\text{Pa}$ )	Method	Reference
Naphthalene (cont'd)	25.0	12.26		
	9–23.91	$\log(p/\text{mmHg}) = 11.7041 - 3798.571/T$	Knudsen effusion method	Radchenko & Kitaigorodskii 74
	9–23.91	$\log(p/\text{Pa}) = 13.83 - 3799/T$	regression from above data	Wania <i>et al.</i> 1994
	–9.54	0.23	diaphragm gauge	Ambrose <i>et al.</i> 1975
	–5.17	0.40		
	0.01	0.74		
	5.07	1.38		
	9.99	2.41		
	14.86	4.13, 4.17		
	20.09	6.93, 6.95		
	25.11	11.35		
	30.14	18.45		
	35.02	28.95		
	40.09	44.73		
	45.06	68.82		
	49.99	104.14		
	55.09	158.41		
	60.24	237.5		
	60.19	238.73, 238.47		
	64.95	340.76		
	69.91	488.58		
	230–344 K	$T \cdot \log(p/\text{Pa}) = \frac{1}{2}a_0 + \sum a_i E_i(x); a_0 = 310.6247,$ $a_1 = 791.4937, a_2 = -82536, a_3 = 0.4043,$ $\log(p/\text{Pa}) = 13.70 - 3773/T$	Chebyshev polynomial	Ambrose <i>et al.</i> 1975
	–20 to 0	$R \cdot \ln(p/\text{mmHg}) = -3351/263.15 + 178.70(1/263.15 - 1/T)$	regression*	from Ambrose <i>et al.</i> 1975
	–20 to 0	$R \cdot \ln(p/\text{mmHg}) = -3351/263.15 + 176.60(1/263.15 - 1/T)$	torsion effusion	de Kruif & van Ginkel 1977
	25	10.64	weighing effusion	de Kruif & van Ginkel 1977
	7.15	1.76	interpolated, Clapeyron eq.	Macknick & Prausnitz 1979
	12.8	3.133	gas saturation	
	18.4	5.586		
	18.85	5.933		
	26.4	12.58		
	31.85	20.53		
	200.3–305 K	$\ln(p/\text{mmHg}) = 26.25 - 8575/T$	Clapeyron eqn., solid	Macknick & Prausnitz 1979
	253–273 K	$\log(p/\text{Pa}) = 14.187 - 3907/T$	torsion effusion, regression	de Kruif 1980
	253–273 K	$\log(p/\text{Pa}) = 14.053 - 3860/T$	weighing effusion, regression	
	253–273 K	$\log(p/\text{Pa}) = 14.107 - 3886/T$	mean regression	
	274.44 K	0.868 temp range 270–385 K	diaphragm manometer	de Kruif <i>et al.</i> 1981
	276.4 K	1.104 (selected from a total of 66 pts)	(pressure sensor)	
	285.37 K	3.02		
	285.71 K	3.11		
	290.88 K	5.35		
	292.75 K	6.5		
	293.83 K	7.29		
	297.4 K	10.42		
	306.67 K	25.27		
	313.96 K	48.67		
	313.88 K	48.94		
	319.58 K	78.38		
	319.59 K	77.9		
	324.05 K	112		
	340.9 K	421.8		
	347.53 K	650		
	345.57 K	653.9		
	352.9 K	941.6		
	353.13 K	969.3		
	274.4–385 K	$R \cdot \ln(p/\text{Pa}) = -\Delta G^\circ(\theta)/\theta + \Delta H^\circ(\theta)(\theta^{-1} - T^{-1}) + \Delta C_{op}(\theta)\{(\theta) - 1 + \ln(T/\theta)\}$ $\theta = 298.15 \text{ K}, \Delta G^\circ(\theta) = -5.989 \text{ kJ mol}^{-1}, \Delta H^\circ(\theta) = 72.51 \text{ kJ mol}^{-1}, \Delta C_{op}^\circ = -57.53 \text{ J K}^{-1} \text{ mol}^{-1}$ $\theta = 373 \text{ K}, \Delta G^\circ(\theta) = -24.16 \text{ kJ mol}^{-1}, \Delta H^\circ(\theta) = 50.246 \text{ kJ mol}^{-1}$	regression*	from de Kruif <i>et al.</i> 1981
	1.20–80.42	$\log(p/\text{Pa}) = 13.59 - 3742/T$	regression*	Colomina <i>et al.</i> 1982
	25	11.41	gas saturation	from Colomina <i>et al.</i> 1982
	–1.68 11.48	$\log(p/\text{Pa}) = 14.01 - 3862/T$	regression*	Grayson & Fosbraey 1982
	28.9	16.38 for temp range 28.9–79 °C	gas saturation	Grayson & Fosbraey 1982
	42.7	58.33		
	50	100.99		

TABLE 3. Vapor pressures and reported equations for temperature dependence of aromatic hydrocarbons—Continued

Compound	$t/^\circ\text{C}$ , $T/\text{K}$ or temp range	Vapor pressure or reported equations: ( $p^s/\text{Pa}$ )	Method	Reference
Naphthalene (cont'd)	60.2	264.32		
	69.6	519.09		
	79	970.5		
	20	6.75		
	302–352 K	$\ln(p/\text{Pa}) = 31.8 - 8753/T$	gas saturation	Grayson & Fosbraey 1982
	302–352 K	$\log(p/\text{Pa}) = 13.83 - 3810/T$	regression*	from Grayson & Fosbraey 1982
	340–752 K	$\log(p/\text{atm}) = (1 - 490.988/T) \times 10^6 (0.832267 - 4.41855 \times 10^{-4} \cdot T + 2.89627 \times 10^{-7} \cdot T^2)$	Cox eq.	Chao <i>et al.</i> 1983
	25	10.4		
	14.15	3.13, 3.24, 3.17		Sonnefeld <i>et al.</i> 1983
	19.49	6.0, 6.19		Bidleman 1984
	25.05	10.1, 10.8, 10.4		Boublík <i>et al.</i> 1984
	32.1	20.9, 21, 20.8		Yamasaki <i>et al.</i> 1984
	10–50	$\log(p/\text{Pa}) = -3960.03/T + 14.299$		Dean 1985
	25	22.64, 28.24		Sato <i>et al.</i> 1986
	80.3–179.5	$\log(p/\text{kPa}) = 6.1638 - 1760.018/(215.204 + t)$	GC-RT, liquid	
	25	17.865 supercooled liquid value	from Fowler <i>et al.</i> 1968	
	126.3–218.6	$\log(p/\text{kPa}) = 5.93404 - 1579.278/(184.062 + t)$	GC retention data	
	86–230	$\log(p/\text{mmHg}) = 7.01065 - 1733.71/(t + 201.86)$	from Camin & Rossini 1955	
	125–218	$\log(p/\text{mmHg}) = 6.8181 - 1585.86/(t + 184.82)$	solid, Antoine eq.	
	25.35	10.7	liquid, Antoine eq.	
	28.35	14.9	gas saturation	
	30.95	19.2		
	34.15	25.9		
	41.65	52.8		
	45.35	71.1		
	48.05	97.5		
	51.85	124		
	55.35	165		
	57.75	200		
	25–57.75	$\ln(p/\text{Pa}) = 22.8929 - 4025.35/(T - 102.343)$	Antoine eq. from exptl data	Sato <i>et al.</i> 1986
	–12.15–70.16	$\log(p/\text{mmHg}) = 10.05263 - 2907.918/(t + 236.459)$	Antoine eq., exptl data	Sasse <i>et al.</i> 1988
	–12.15	0.165	pressure gauge	
	–9.47	0.227		
	0.52	0.820		
	10.17	2.413		
	20.1	7.09, 7.03		
	30.0	18.26, 18.80		
	40.04	44.93, 45.46		
	50.04	106.8, 105.2		
	60.05	238, 232.6		
	70.2	491, 500		
	80.16–90.15	$\log(p/\text{mmHg}) = 2.25180 - 76.496/(t - 25.02)$	Antoine eq., exptl data, liq.	
	80.16	969, 973 liquid state	pressure gauge	Sasse <i>et al.</i> 1988
	84.9	1240		
	87.2	1383, 1396		
	90.15	1590.5		
	25	41.88, 38.02 supercooled liquid value	GC retention data, liquid	Hinckley <i>et al.</i> 1990
	–36 to 0	$\log(p/\text{Pa}) = 13.93 - 3851/T$	gas saturation-GC	Wania <i>et al.</i> 1994
	recommended value at 25 °C: 10.4 ± 1.0 Pa			
1-Methylnaphthalene	142.1–245.4	$\log(p/\text{mmHg}) = 7.03592 - 1826.948/(195.002 + t)$	Antoine eq. from exptl data	Camin & Rossini 1955
	108–278	$\log(p/\text{mmHg}) = 7.03592 - 1826.948/(195.002 + t)$	Antoine eq.	Zwolinski & Wilhoit 1971
	5.7	1.760 temp range 5.7–38.6 °C	gas saturation	Macknick & Prausnitz 1979
	11.4	2.920		
	18.1	5.248		
	22.15	7.133		
	28.85	12.59		
	32.25	15.732		
	34.9	18.931		
	38.6	23.464		
	5.7–38.6	$\ln(p/\text{mmHg}) = 20.552 - 6933.2/T$	Clapeyron eq., exptl data	Macknick & Prausnitz 1979
	279–593 K	$\log(p/\text{atm}) = (1 - 517.727/T) \times 10^6 (0.863323 - 6.26356 \times 10^{-4} \cdot T + 3.75850 \times 10^{-7} \cdot T^2)$	Cox eq.	Chao <i>et al.</i> 1983
	141–245.3	$\log(p/\text{kPa}) = 6.15917 - 1825.586/(244.686 + t)$	data of Camin & Rossini	Boublík <i>et al.</i> 1984
	25	7.43, 6.31	GC-RT liquid	Budkenab 1874

TABLE 3. Vapor pressures and reported equations for temperature dependence of aromatic hydrocarbons—Continued

Compound	<i>t</i> /°C, <i>T</i> /K or temp range	Vapor pressure or reported equations: ( <i>p</i> <sup>5</sup> /Pa)	Method	Reference
1-Methylnaphthalene (cont'd)	108–278 278–313 K 415–526 K –14.4–115.1 –14.44 –9.64 10.14 20.18 30.15 40.04 49.90 59.89 69.98 79.94 89.99 100.06 110.04 115.10 25	$\log(p/\text{mmHg}) = 7.03592 - 1826.948/(t + 195.00)$ $\log(p/\text{kPa}) = 7.03469 - 3006.267/T$ $\log(p/\text{kPa}) = 6.15928 - 1826.402/(-78.176 + T)$ $\log(p/\text{mmHg}) = 7.27126 - 2006.662/(t + 212.625)$ 0.189 liquid phase 0.317 2.386 6.093 13.73 28.40 56.53 107.2 193.7 342.4 578.6 950 1507 1888 8.83 supercooled liquid value recommended value at 25 °C: 8.84 ± 0.40 Pa	Antoine eq. Antoine eq., liquid Antoine eq., liquid pressure gauge, exptl data pressure gauge	Dean 1985 Stephenson & Malanowski 1987 Stephenson & Malanowski 1987 Sasse <i>et al.</i> 1988
2-Methylnaphthalene	139.1–242 105–274.4 378–629 K 139–242 105–274 423–515 K	$\log(p/\text{mmHg}) = 7.06850 - 1840.268/(198.395 + t)$ $\log(p/\text{mmHg}) = 7.06850 - 1840.268/(198.395 + t)$ $\log(p/\text{atm}) = (1 - 514.242/T) \times 10^{-6} (0.879050 - 5.85793 \times 10^{-4} \cdot T + 4.19253 \times 10^{-7} \cdot T^2)$ $\log(p/\text{kPa}) = 6.19639 - 1842.831/(198.592 + t)$ $\log(p/\text{mmHg}) = 7.06850 - 1840.288/(t + 198.40)$ $\log(p/\text{kPa}) = 6.21475 - 1858.19/(-72.779 + T)$ recommended value at 25 °C: 9.0 Pa	Antoine eq. from exptl. data Antoine eq. Cox eq. data of Camin & Rossini Antoine eq. Antoine eq., liquid	Camin & Rossini 1955 Zwolinski & Wilhoit 1971 Chao <i>et al.</i> 1983 Boublik <i>et al.</i> 1984 Dean 1985 Stephenson & Malanowski 1987
1-Ethylnaphthalene	120–292 393–565 K 393–565 K	$\log(p/\text{mmHg}) = 7.03159 - 1841.320/(185.28 + t)$ $\log(p/\text{atm}) = (1 - 531.480/T) \times 10^{-6} (0.923623 - 6.97505 \times 10^{-4} \cdot T + 5.07450 \times 10^{-7} \cdot T^2)$ $\log(p/\text{kPa}) = 6.15645 - 1841.32/(-87.87 + T)$ recommended value at 25 °C: 2.51 Pa	Antoine eq. Cox eq. Antoine eq., liquid	Zwolinski & Wilhoit 1971 Chao <i>et al.</i> 1983 Stephenson & Malanowski 1987
2-Ethylnaphthalene	119–292 70–258.1 13.05 17.9 22.9 29.5 34.85 39.4 45.1 13.05–45.1 286–565 K 286–319 K 393–565 K –4.65–125 –4.65 0.26 10.17 20.1 30.11 40.01 49.91 59.92 69.96 79.98 90.01 100.08 110.08 120.02	$\log(p/\text{mmHg}) = 7.07566 - 1880.73/(191.41 + t)$ $\log(p/\text{mmHg}) = (-0.2185 \times 12751.3/T) + 8.138798$ 1.533 measured range 13.05–45.1 °C 2.213 3.400 6.213 9.799 13.159 19.998 $\ln(p/\text{mmHg}) = 21.485 - 7435.9/T$ $\log(p/\text{atm}) = (1 - 531.189/T) \times 10^{-6} (0.871612 - 5.23140 \times 10^{-4} \cdot T + 3.70623 \times 10^{-7} \cdot T^2)$ $\log(p/\text{kPa}) = 7.46683 - 3232.791/T$ $\log(p/\text{kPa}) = 6.20056 - 1880.73/(-82.74 + T)$ $\log(p/\text{mmHg}) = 6.83541 - 1799.779/(t + 189.505)$ 0.164 liquid phase 0.30 0.880 2.426, 2.40 6.05 13.33 27.33 54.26 103.6 187.9 326.8 551.8 898.1 1420 recommended value at 25 °C: 4.0 ± 0.30 Pa	Antoine eq. Antoine eq. gas saturation Clapeyron eq. from expt. Cox eq. Antoine eq., liquid Antoine eq., liquid Antoine eq., exptl data Macknick & Prausnitz 1979 Chao <i>et al.</i> 1983 Stephenson & Malanowski 1987 Sasse <i>et al.</i> 1988 Macknick & Prausnitz 1979 Stephenson & Malanowski 1987 Sasse <i>et al.</i> 1988	Zwolinski & Wilhoit 1971 Weast 1972–73 Macknick & Prausnitz 1979 Macknick & Prausnitz 1979 Chao <i>et al.</i> 1983 Stephenson & Malanowski 1987 Stephenson & Malanowski 1987 Sasse <i>et al.</i> 1988
1,2-Dimethylnaph.	129–268	$\log(p/\text{mmHg}) = 7.00605 - 1805.31/(171.37 + t)$ recommended value at 25 °C: 0.87 Pa	Antoine eq.	Zwolinski & Wilhoit 1971

TABLE 3. Vapor pressures and reported equations for temperature dependence of aromatic hydrocarbons—Continued

Compound	<i>t</i> /°C, <i>T</i> /K or temp range	Vapor pressure or reported equations: ( <i>p</i> <sup>s</sup> /Pa)	Method	Reference
1,3-Dimethylnaph.	400–541 K	$\log(p/\text{atm}) = (1 - 540.353/T) \times 10^{-4} (1.72680 - 7.87991 \times 10^{-4} \cdot T - 42.8535 \times 10^{-7} \cdot T^2)$	Cox eq.	Chao <i>et al.</i> 1983
	20–148	$\log(p/\text{mmHg}) = 7.6347 - 2345.4/(t + 232.8)$	Antoine eq.	Dean 1985
	148–310	$\log(p/\text{mmHg}) = 7.2698 - 2075.0/(t - 210)$ recommended value at 25 °C:		
1,4-Dimethylnaph.	397–544 K	$\log(p/\text{atm}) = (1 - 544.363/T) \times 10^{-4} (1.97594 - 8.55425 \times 10^{-4} \cdot T - 51.4189 \times 10^{-7} \cdot T^2)$	Cox eq.	Chao <i>et al.</i> 1983
	20–148	$\log(p/\text{mmHg}) = 7.6347 - 2345.8/(t + 232.6)$	Antoine eq.	Dean 1985
	148–310	$\log(p/\text{mmHg}) = 7.2698 - 2076.0/(t + 210)$		
1,6-Dimethylnaph.	328–415 K	$\log(p/\text{atm}) = (1 - 687.081/T) \times 10^{-4} (1.14901 - 11.9220 \times 10^{-4} \cdot T - 17.3468 \times 10^{-7} \cdot T^2)$	Cox eq.	Chao <i>et al.</i> 1983
	111–145	$\log(p/\text{kPa}) = 5.19014 - 1325.209/(139.781 + t)$	Osborn & Douslin 1966 data	Boublik <i>et al.</i> 1984
	20–150	$\log(p/\text{mmHg}) = 7.3968 - 2080.3/(t + 200.8)$	Antoine eq., solid	Dean 1985
	150–310	$\log(p/\text{mmHg}) = 7.0460 - 1841/(t + 180)$	Antoine eq., liquid	
	278–304 K	$\log(p/\text{kPa}) = 11.290 - 4386.4/T$	Antoine eq., solid	Stephenson & Malanowski 1987
	348–383 K	$\log(p/\text{kPa}) = 8.45107 - 2512.509/(-89.765 + T)$	Antoine eq., solid	
	384–418 K	$\log(p/\text{kPa}) = 5.18084 - 1320.21/(-133.876 + T)$	Antoine eq., liquid	
	recommended value at 25 °C: 2.27 Pa			
	328–413 K	$\log(p/\text{atm}) = (1 - 576.908/T) \times 10^{-4} (0.951477 - 8.49048 \times 10^{-4} \cdot T + 2.61743 \times 10^{-7} \cdot T^2)$	Cox eq.	Chao <i>et al.</i> 1983
1,8-Dimethylnaph.	65–140	$\log(p/\text{kPa}) = 6.5446 - 2195.436/(209.114 + t)$	Osborn & Douslin 1966 data	Boublik <i>et al.</i> 1984
	25–150	$\log(p/\text{mmHg}) = 7.40789 - 2123.2/(t + 201.2)$	Antoine eq.	Dean 1985
	150–320	$\log(p/\text{mmHg}) = 7.0564 - 1879/(t + 180)$		
	328–336 K	$\log(p/\text{kPa}) = 10.56808 - 4066.836/T$	Antoine eq., solid	Stephenson & Malanowski 1987
	338–547 K	$\log(p/\text{kPa}) = 6.54778 - 2197.524/(-63.88 + T)$ recommended value at 25 °C:	Antoine eq., liquid	Stephenson & Malanowski 1987
2,3-Dimethylnaph.	333–408 K	$\log(p/\text{atm}) = 631.969/T \times 10^{-4} (1.09999 - 10.2378 \times 10^{-4} \cdot T - 11.3931 \times 10^{-7} \cdot T^2)$	Cox eq.	Chao <i>et al.</i> 1983
	105–135	$\log(p/\text{kPa}) = 5.27335 - 1383.083/(141.333 + t)$	Osborn & Douslin 1966 data	Boublik <i>et al.</i> 1984
	20–155	$\log(p/\text{mmHg}) = 7.40396 - 2111.9/(t - 201.1)$	Antoine eq., solid	Dean 1985
	165–315	$\log(p/\text{mmHg}) = 7.0527 - 1869/(t + 180)$	Antoine eq., liquid	
	278–304 K	$\log(p/\text{kPa}) = 10.625 - 4172.6/T$	Antoine eq., solid	Stephenson & Malanowski 1987
	333–373 K	$\log(p/\text{kPa}) = 8.97897 - 2959.733/(-59.936 + T)$	Antoine eq., solid	
	378–408 K	$\log(p/\text{kPa}) = 5.57091 - 1544.764/(-116.821 + T)$ recommended value at 25 °C: 1.0 Pa	Antoine eq., liquid	
2,7-Dimethylnaph.	333–398 K	$\log(p/\text{atm}) = (1 - 632.459/T) \times 10^{-4} (1.11518 - 10.6526 \times 10^{-4} \cdot T - 13.2234 \times 10^{-7} \cdot T^2)$	Cox eq.	Chao <i>et al.</i> 1983
	96–125	$\log(p/\text{kPa}) = 6.46533 - 2082.408/(206.164 + t)$	Osborn & Douslin 1966 data	Boublik <i>et al.</i> 1984
	25–150	$\log(p/\text{mmHg}) = 7.39875 - 2085.9/(t + 200.9)$	Antoine eq., solid	Dean 1985
	150–310	$\log(p/\text{mmHg}) = 7.0478 - 1846/(t + 280)$	Antoine eq., liquid	
	323–368 K	$\log(p/\text{kPa}) = 9.40197 - 3047.828/(-58.898 + T)$	Antoine eq., solid	Stephenson & Malanowski 1987
	369–535 K	$\log(p/\text{kPa}) = 6.4818 - 2092.928/(-66.181 + T)$ recommended value at 25 °C:	Antoine eq., liquid	
Biphenyl	4.9–34.5	$\log(p/\text{mmHg}) = 10.38 - 3799/T$	effusion	Bright 1951
	15.05	measured temp range 15–41 °C	effusion	Bradley & Cleasby 1953
	20.7	0.7786		
	24.7	1.2252		
	24	1.1825		
	24.1	1.1839		
	27.05	1.5998		
	29.15	2.0531		
	32.45	2.9730		
	35.05	3.8663		
	37.9	5.1595		
	40.55	6.6927		
	23.05	1.0266		
	36.5	1.5332		Weast 1972–73
	31.25	2.5464		Radchenko & Kitagorodskii 74
	35.9	4.1329		
	15–41	$\log(p/\text{mmHg}) = 11.282 - 4262/T$	effusion	Bradley & Cleasby 1953
	70.6–254.9	$\log(p/\text{mmHg}) = (-0.2185 \times 129.10/T) + 8.218583$	Antoine eq.	
	24.9	temp range 24.9–50 °C	Knudsen effusion method	
	31.75	2.976		

TABLE 3. Vapor pressures and reported equations for temperature dependence of aromatic hydrocarbons—Continued

Compound	<i>t</i> /°C, <i>T</i> /K or temp range	Vapor pressure or reported equations: ( <i>p</i> <sup>s</sup> /Pa)	Method	Reference
Biphenyl (cont'd)	33.7	3.734		
	35.5	4.538		
	37.6	5.726		
	39.57	6.913		
	41.52	8.259		
	43.48	10.259		
	45.45	12.349		
	47.4	15.492		
	50	1.946		
	24.9–50	$\log(p/\text{mmHg}) = 12.6789 - 4367.436/T$	Knudsen effusion method	Radchenko & Kitaigorodskii 74
	5.2	0.106 measured temp range 5.2–24.7 °C	gas saturation	Burkhard <i>et al.</i> 1984
	14.9	0.361		
	24.7	1.15		
	5.2–24.7	$\log(p/\text{Pa}) = 14.840 - 4402.1/T$	gas saturation	Burkhard <i>et al.</i> 1984
	25	2.86 supercooled liquid value	GC retention data	Yamasaki <i>et al.</i> 1984
	69.2–271	$\log(p/\text{kPa}) = 6.368\ 95 - 1997.558/(202.608 + t)$	Antoine eq.	Boublik <i>et al.</i> 1984
	69–271	$\log(p/\text{mmHg}) = 7.245\ 41 - 1998.723(t + 202.733)$	Antoine eq.	Dear 1985
	297–324 K	$\log(p/\text{kPa}) = 11.719\ 29 - 4341.054/T$	Antoine eq., solid	Stephenson & Malanowski 1987
	283–342 K	$\log(p/\text{kPa}) = 28.5175 - 21141.5/(374.85 + T)$	Antoine eq., solid	
	390–563 K	$\log(p/\text{kPa}) = 6.375\ 26 - 1974.8/(-75.85 + T)$	Antoine eq., liquid	
	25	5.61, 5.00	GC retention data, liquid	Hinckley <i>et al.</i> 1990
	25	3.35, 3.41	GC retention data, liquid	Bidleman 1984
	recommended value at 25 °C: <i>p</i> <sup>s</sup> =1.30 Pa			
Diphenylmethane	76–264.5	$\log(p/\text{mmHg}) = (-0.2185 \times 13089.4/T) + 8.215927$	Antoine eq.	Weast 1972-73
	217.5–282	$\log(p/\text{kPa}) = 5.387\ 01 - 1240.329/(102.464 + t)$	Antoine eq.	Boublik <i>et al.</i> 1984
	295–383 K	$\log(p/\text{kPa}) = 5.8765 - 1707.9/(-101.15 + T)$	Antoine eq., liquid	Stephenson & Malanowski 1987
	423–583 K	$\log(p/\text{kPa}) = 6.286\ 15 - 1944.42/(-83.15 + T)$	Antoine eq., liquid	
	recommended value at 25 °C: 0.0885 Pa			
1,1-Diphenylethane	348–405 K	$\log(p/\text{kPa}) = 8.884\ 69 - 3261.481/T$	Antoine eq., liquid	Stephenson & Malanowski 1987
	recommended value at 25 °C			
Bibenzyl	86.8–284	$\log(p/\text{mmHg}) = (-0.2185 \times 13387.6/T) + 8.142488$	Antoine eq.	Weast 1972-73
(1,2-Diphenylethane)	286–308 K	$\log(p/\text{kPa}) = 11.319 - 4386/T$	Antoine eq., solid	Stephenson & Malanowski 1987
	359–557 K	$\log(p/\text{kPa}) = 6.93271 - 2636.21/(-22.009 + T)$	Antoine eq., liquid	
	recommended value at 25 °C: 0.406 Pa			
1,1-Diphenylethylene	87.4–277	$\log(p/\text{mmHg}) = (-0.2188 \times 13\ 778.1/T) + 8.369088$	Antoine eq.	Weast 1972-73
	360–550 K	$\log(p/\text{kPa}) = 6.915\ 64 - 2522.93/(-35.439 + T)$	Antoine eq., liquid	Stephenson & Malanowski 1987
	recommended value at 25 °C			
<i>cis</i> -Stilbene				
(1,2-Diphenylethylene, <i>cis</i> )	373–428 K	$\log(p/\text{kPa}) = 8.609 - 3474/T$	Antoine eq., liquid	Stephenson & Malanowski 1987
<i>trans</i> -Stilbene	113.2–306.5	$\log(p/\text{mmHg}) = (-0.2185 \times 15015.1/T) + 8.529\ 650$	Antoine eq.	Weast 1972-73
1,2-Diphenylethylene, <i>trans</i> -	25	0.00765	spinning rotor friction gauge	Van Ekeren <i>et al.</i> 1983
	24.35–43.35	$R \ln(p/\text{kPa}) = -12064/\theta + 100.7[1/(1/\theta - 1/T)], \theta = 298.15\ K$	spinning rotor friction gauge	Van Ekeren <i>et al.</i> 1983
	24.3	0.007 04, 0.006 99, 0.007 15	spinning rotor friction gauge	Van Ekeren <i>et al.</i> 1983
	24.43	0.006 93		
<i>trans</i> -Stilbene (cont'd)	27.24	0.0102, 0.0104, 0.0105		
	30.65	0.0151, 0.015		
	32.03	0.0196, 0.0195		
	34.96	0.0287, 0.0288, 0.0289		
	37.33	0.0386, 0.0387		
	40.61	0.0584, 0.0585		
	43.32	0.0792		
	44.97	0.100	torsion mass loss effusion	Van Ekeren <i>et al.</i> 1983
	50.78	0.200		
	54.27	0.300		
	56.8	0.400		
	58.79	0.500		
	60.43	0.600		
	64.14	0.900		

TABLE 3. Vapor pressures and reported equations for temperature dependence of aromatic hydrocarbons—Continued

Compound	<i>t</i> /°C, <i>T</i> /K or temp range	Vapor pressure or reported equations: ( <i>p</i> <sup>s</sup> /Pa)	Method	Reference
<i>trans</i> -Stilbene (cont'd)	65.11	1.000		
	69.45	1.44		
	71.25	1.83, 1.80		
	72.2	1.94		
	73.7	2.25		
	74.18	2.39		
	75.73	2.81		
	75.86	2.83		
	76.88	3.10		
	78.27	3.55		
	80.39	4.39		
	81.79	5.07		
	83.36	5.84		
	85.04	6.86		
	86.35	7.71		
	86.51	7.90		
	87.35	8.47		
	89.74	10.57		
	90.43	11.22		
	91.35	12.20		
	307.8 K	0.0274	quartz-crystal balance	Offringa <i>et al.</i> 1983
	recommended value at 25 °C: <i>p</i> <sup>s</sup> =0.0077 Pa			
Acenaphthylene	11.2	0.206, 0.205, 0.216 measured range 11.2–39 °C	gas saturation	Sonnefeld <i>et al.</i> 1983
	20.56	0.590, 0.585, 0.588		
	30.4	1.50, 1.54, 1.52		
	39.05	3.30, 3.41, 3.27, 3.34		
	25	0.89		
	10–50	$\log(p/\text{Pa})=12.768-3821.55/T$	gas saturation	Sonnefeld <i>et al.</i> 1983
	recommended value at 25 °C: <i>p</i> <sup>s</sup> =0.90 Pa			
Acenaphthene	147–288	$\log(p/\text{mmHg})=8.033-2835/T$	static isoteniscope method	Mortimer & Murphy 1923
	–15–35	$\log(p/\text{mmHg})=11.50-4264/T$	effusion	Hoyer & Peperle 1958
	114.8–278	$\log(p/\text{mmHg})=(-0.2185 \times 13078.5/T) + 8.069478$	Antoine eq.	Weast 1972–73
	54.1	8.622 temp range 54.1–83.45 °C	effusion method	Radchenko & Kitaigorodskii 74
	57.85	10.376		
	58.95	13.180		
	61.3	16.545		
	64.55	20.438		
	67.25	26.757		
	69.5	31.304		
	71.8	37.770		
	73.65	47.222		
	76	57.234		
	78.05	67.660		
	80.5	82.045		
	83.45	130.296		
	54–83.45	$\log(p/\text{mmHg})=12.2930-4222.924/T$		Radchenko & Kitaigorodskii 74
	65	25.865 measured temp range 65–93.195 °C	inclined-piston manometry	Osborn & Douslin 1975
	70	30.797		
	75	46.796		
	80	70.526		
	85	104.92		
	90	153.45		
	92.5	185.05		
	93.195	195.05		
	95	214.91 measured range 95–140.95 °C	inclined-piston manometry	Osborn & Douslin 1975
	100	281.04		
	105	364.23		
	110	468.35		
	115	597.94		
	120	755.39		
	125	948.97		
	130	1184		
	135	1469		
	140	1809		
	10.87	0.048, 0.0504, 0.0515 measured temp range 11–40 °C	gas saturation	Sonnefeld <i>et al.</i> 1983
	20.45	0.167, 0.161, 0.166		

TABLE 3. Vapor pressures and reported equations for temperature dependence of aromatic hydrocarbons—Continued

Compound	<i>t</i> /°C, <i>T</i> /K or temp range	Vapor pressure or reported equations: ( <i>p</i> <sup>s</sup> /Pa)	Method	Reference
Acenaphthene (cont'd)	30.15	0.539, 0.512		
	32.15	0.580		
	38.9	1.35, 1.32, 1.32		
	25	0.287		
	10–50	$\log(p/\text{Pa}) = 14.669 - 4335.39/T$	gas saturation	Sonnefeld <i>et al.</i> 1983
	25	1.009 supercooled liquid value	GC retention data	Yamasaki <i>et al.</i> 1984
	95–140	$\log(p/\text{kPa}) = 6.385 \cdot 04 - 2102.491/(203.124 + t)$	Osborn & Douslin 1966 data	Boublik <i>et al.</i> 1984
	147–288	$\log(p/\text{kPa}) = 6.845 \cdot 71 - 2527.716/(244.912 + t)$	Mortimer & Murphy 1923	Boublik <i>et al.</i> 1984
	147–183	$\log(p/\text{mmHg}) = 7.728 \cdot 19 - 2534.234/(t + 245.576)$	Antoine eq.	Dean 1985
	147–288	$\log(p/\text{mmHg}) = 8.033 - 2834.99/T$	Antoine eq.	Dean 1985
	19.95	0.237	gas saturation	Sato <i>et al.</i> 1986
	26.85	0.319		
	30.85	0.792		
	35.75	1.30		
	37.95	1.60		
	43.35	3.21		
	45.35	4.23		
	48.35	5.76		
	51.85	7.68		
	58.05	9.72		
	60.25	12.0		
	63.65	15.6		
	68.85	23.5		
	293.1–342 K	$\log(p/\text{Pa}) = 22.9288 - 5183.86/(T - 80.153)$	Antoine eq., gas satn data	Sato <i>et al.</i> 1986
	290–311 K	$\log(p/\text{kPa}) = 10.883 - 4290.5/T$	Antoine eq., solid	Stephenson & Malanowski 1987
	338–366 K	$\log(p/\text{kPa}) = 9.4944 - 3248.008/T$	Antoine eq., solid	
	368–413 K	$\log(p/\text{kPa}) = 6.3539 - 2082.356/(-71.578 + T)$	Antoine eq., liquid	
	388–552 K	$\log(p/\text{kPa}) = 7.304 \cdot 01 - 2975/(10.674 + T)$	Antoine eq., liquid	
recommended value at 25 °C: <i>p</i> <sup>s</sup> =0.30±0.030 Pa				
Fluorene	161–300.4	$\log(p/\text{mmHg}) = 8.059 - 2957/T$	static isotenoscope method	Mortimer & Murphy 1923
	33.3	0.2186 measured temp range 33–50 °C	effusion	Bradley & Cleasby 1953
	37.2	0.3333		
	40.3	0.4573		
	45	0.7239		
	49.25	1.0906		
	34.85	0.2600		
	38.45	0.3746		
	42.45	0.5546		
	47.75	0.9439		
	49.55	1.1106		
	33–50	$\log(p/\text{mmHg}) = 10.325 - 4324/T$	effusion	Bradley & Cleasby 1953
	129.3–295	$\log(p/\text{mmHg}) = (-0.2185 \times 13682.8/T) + 8.128894$	Antoine eq.	Weast 1972–73
	75	15.065 for temp range 75–114 °C	inclined-piston manometry	Osborn & Douslin 1975
	80	22.264		
	85	32.263		
	90	47.462		
	95	68.26		
	100	99.19		
	105	141.45		
	110	199.98		
	114	259.041		
	10.5	0.0132, 0.0133, 0.013	gas saturation-HPLC	Sonnefeld <i>et al.</i> 1983
	20.4	0.0425, 0.438, 0.0451		
	30	0.147		
	29.97	0.153, 0.146		
	38.85	0.387, 0.384, 0.382		
	38.9	0.387, 0.393		
	25	0.080		
	10–50	$\log(p/\text{Pa}) = 14.385 - 4616.07/T$	gas saturation data	Sonnefeld <i>et al.</i> 1983
	25	0.408	GC retention data, liquid	Yamasaki <i>et al.</i> 1984
	161–300.4	$\log(p/\text{kPa}) = 6.884 \cdot 99 - 2635.471/(743.022 + t)$	from Mortimer & Murphy	Boublik <i>et al.</i> 1984
	25	0.473, 0.380	GC retention data, liquid	Bidleman 1984
	161–300	$\log(p/\text{mmHg}) = 7.7618 - 2637.1/(t + 243.2)$	Antoine eq.	Dean 1985
	34.55	0.297	gas saturation method	Sato <i>et al.</i> 1986
	36.35	0.360		

TABLE 3. Vapor pressures and reported equations for temperature dependence of aromatic hydrocarbons—Continued

Compound	t/°C, T/K or temp range	Vapor pressure or reported equations: (p <sup>s</sup> /Pa)	Method	Reference
Fluorene (cont'd)	41.15	0.630		
	47.45	1.210		
	49.85	1.53		
	52.35	1.95		
	57.35	3.07		
	62.35	4.78		
	67.25	7.38		
	71.25	10.20		
	74.35	13.0		
	34.5–74.35	$\ln(p/\text{Pa}) = 17.0935 - 2185.52/(T - 153.984)$	Antoine eq. from exptl data	Sato <i>et al.</i> 1986
	306–323 K	$\log(p/\text{kPa}) = 10.449 - 4234/T$	Antoine eq., solid	Stephenson & Malanowski 1987
	348–388 K	$\log(p/\text{kPa}) = 10.04542 - 4122.908/T$	Antoine eq., solid	
	420–568 K	$\log(p/\text{kPa}) = 8.31368 - 4133.08/(86.582 + T)$	Antoine eq., liquid	
	30.03	0.157	pressure gauge	Sasse <i>et al.</i> 1988
	39.93	0.184		
	49.88	1.241		
	59.92	3.426		
	60.03	3.533		
	69.93	8.746		
	79.98	20.67, 20.8		
	99.99	46.40		
	100.08	99.06, 98.93		
	30–100.08	$\log(p/\text{mmHg}) = 11.64431 - 4268.644/(262.656 + t)$	Antoine eq., for solid	
	100–154.8	$\log(p/\text{mmHg}) = 7.94839 - 2641.73/(t + 230.963)$	Antoine eq., for liquid	Sasse <i>et al.</i> 1988
	110.06	212.5 liquid phase	pressure gauge	
	120.04	352, 353		
	129.97	568.6		
	139.95	894.3		
	149.86	1368.6		
	154.81	1683		
	25	0.793, 0.652 supercooled liquid value recommended value at 25 °C: p <sup>s</sup> =0.09±0.01 Pa	GC retention data, liquid	Hinckley <i>et al.</i> 1990
Anthracene	100–350	$\log(p/\text{mmHg}) = 10.972 - 4594/T$	Antoine eq., solid	Mortimer & Murphy 1923
	232–340.5	$\log(p/\text{mmHg}) = 7.910 - 3093/T$	static isoteniscope method	Mortimer & Murphy 1923
	105–125	$\log(p/\text{mmHg}) = 12.002 - 5102.0/T$	Rodebush gage	Sears & Hopke 1949
	25	0.00103	extrapolated effusion, anthracene I	Inokuchi <i>et al.</i> 1952
		$\log(p/\text{mmHg}) = 11.420 - 4795.0/T$ , mean exptl temp 91 °C	effusion, anthracene II	
		$\log(p/\text{mmHg}) = 11.611 - 4820/T$ , mean exptl temp 92 °C	effusion	Bradley & Cleasby 1953
	65.7	0.115 measured temp range 66–80.4 °C		
	69.91	0.167		
	73.55	0.259		
	77.25	0.308		
	79.95	0.489		
	67.1	0.140		
	68.75	0.157		
	71.25	0.208		
	73.2	0.223		
	80.4	0.524		
	66–80.4	$\log(p/\text{mmHg}) = 11.638 - 5320/T$	effusion	Bradley & Cleasby 1953
	123–148	$\log(p/\text{mmHg}) = 12.002 - 5102/T$	fluorescence	Stevens 1953
	30–100	$\log(p/\text{mmHg}) = 11.150 - 5401/T$	effusion	Hoyer & Peperle 1958
	105–125	2.00 measured temp range 95–105 °C 2.853 4.333	interpolated data	Kelley & Rice 1964
	105–105	1.587 measured temp range 95–105 °C 2.466 3.773	interpolated data of Klochkov	Kelley & Rice 1964
	69–86	$\log(p/\text{mmHg}) = 12.068 - 5145/T$	effusion	Kelley & Rice 1964
	69–86	1.667	extrapolated from above eq.	
	69–86	2.546		
	69–86	3.88		
	175.5–380	$\log(p/\text{mmHg}) = 7.67401 - 2819.63/(247.01 + t)$	Antoine eq., liquid	Zwolinski & Wilhoit 1971
	100–600	$\log(p/\text{mmHg}) = (-0.2185 \times 16)823.6/T + 8.70600$	Antoine eq.	Weast 1972–73

TABLE 3. Vapor pressures and reported equations for temperature dependence of aromatic hydrocarbons—Continued

Compound	<i>t</i> /°C, <i>T</i> /K or temp range	Vapor pressure or reported equations: ( <i>p</i> <sup>S</sup> /Pa)	Method	Reference
Anthracene (cont'd)	79.5–159	$\log(p/\mu\text{mmHg}) = 12.616 - 5277/T$ 0.612	Knudsen effusion	Malaspina <i>et al.</i> 1977
	79.55	1.373		
	88.25	3.506		
	98.05	6.413		
	105.95	12.17		
	113.75	29.33		
	123.75	61.06		
	135.25	106.52		
	142.35	189.31		
	149.75	483.95		
	159.15			
	30–100	$\log(p/\mu\text{mmHg}) = 36.40 - 8634/(t + 238.6)$ 0.009 37	regression, gas saturation-GC gas saturation-GC	Power <i>et al.</i> 1977
	30	0.009 13		
	30	0.0928		
	50	0.582		
	70	0.5826		
	70	7.338		
	100	7.771		
	85.25	0.892 measured temp range 85–120 °C	gas saturation	Macknick & Prausnitz 1979
	90.15	1.36		
	95.65	2.13		
	100.7	3.32		
	104.7	4.59		
	111.9	8.04		
	116.4	11.41		
	119.95	14.67		
	85–120	$\ln(p/\text{mmHg}) = 26.805 - 11402/T$	Clapeyron eq., solid	Macknick & Prausnitz 1979
	338–391 K	$\log(p/\text{Pa}) = 14.577 - 5254/T$	torsion-effusion	de Kruif 1980
	338–391 K	$\log(p/\text{Pa}) = 14.457 - 5217.5/T$	weighing-effusion	
	338–391 K	$\log(p/\text{Pa}) = 14.529 - 5243.6/T$	mean value	
	25	0.000 75	extrapolated	de Kruif 1980
	50.1	0.035 for temp range 50.1–80.5 °C	gas saturation	Grayson & Fosbraey 1982
	60	0.0849		
	70	0.267		
	75	0.359		
	80.5	0.588		
	20	0.001 02		
	50.1–80.5	$\ln(p/\text{Pa}) = 30.5 - 10968/T$		Grayson & Fosbraey 1982
	12.3	$(1.64, 1.57, 1.60) \times 10^{-4}$ temp range 12.3–50 °C	gas saturation	Sonnefeld <i>et al.</i> 1983
	19.2	$(3.76, 3.82, 3.54, 3.72) \times 10^{-4}$		
	25	$(8.43, 8.17, 8.19, 8.3) \times 10^{-4}$		
	30.1	$(1.46, 1.54, 1.51) \times 10^{-3}$		
	34.93	$(2.59, 2.63, 2.69) \times 10^{-3}$		
	10–50	$\log(p/\text{Pa}) = 12.977 - 4791.87/T$	gas saturation	Sonnefeld <i>et al.</i> 1983
	80.45	0.55 measured temp range 80–125 °C	gas saturation	Bender <i>et al.</i> 1983
	82.05	0.67		
	85.35	0.864		
	90.5	1.418		
	94.5	2.019		
	100.8	3.426		
	105.65	4.99		
	110.4	7.17		
	115.35	10.01		
	115.65	10.58		
	110.85?	15.3		
	125.45	21.3		
	80–125	$\ln(p/\text{Pa}) = 31.620 - 1138/T$	gas saturation	Bender <i>et al.</i> 1983
	25	0.066 supercooled liquid value	GC retention data	Yamasaki <i>et al.</i> 1984
	220–310	$\log(p/\text{kPa}) = 6.66266 - 2659.55/(230.119 + t)$	Antoine eq.	Boublik <i>et al.</i> 1984
	223–340.5	$\log(p/\text{kPa}) = 6.53182 - 2550.737/(221.756 + t)$	Antoine eq.	Boublik <i>et al.</i> 1984
	100–160	$\log(p/\text{mmHg}) = 8.91 - 3761/T$	Antoine eq., solid	Dean 1985
	176–380	$\log(p/\text{mmHg}) = 7.67401 - 2819.63/(t + 247.02)$	Antoine eq., liquid	Dean 1985
	25	0.00106	gas saturation-GC	Rordorf 1985
	50	0.023		
	75	0.322		
	100	3.17		

TABLE 3. Vapor pressures and reported equations for temperature dependence of aromatic hydrocarbons—Continued

Compound	<i>t</i> /°C, <i>T</i> /K or temp range	Vapor pressure or reported equations: ( <i>p</i> <sup>s</sup> /Pa)	Method	Reference
Anthracene (cont'd)	125	23.4		
	150	136.2		
	313.15 K	0.0058	gas saturation-IR	Hansen & Eckert 1986
	318.15 K	0.0105		
	323.15 K	0.0193		
	328.15 K	0.039		
	333.15 K	0.0675		
	338.15 K	0.0987		
	343.15 K	0.1688		
	348.15 K	0.3056		
	353.16 K	0.5252		
	358.15 K	0.9147		
	363.15 K	1.244		
	313–363 K	$\log(p/\text{mPa}) = 17.88 - 5359/T$		Hansen & Eckert 1986
	299–430 K	$\log(p/\text{kPa}) = 10.58991 - 4903.3/T$	Antoine eq., solid	Stephenson & Malanowski 1987
	313–363 K	$\log(p/\text{kPa}) = 11.76139 - 5315.532/T$	Antoine eq., solid	
	363–393 K	$\log(p/\text{kPa}) = 10.75544 - 4947.951/T$	Antoine eq., solid	
	504–613 K	$\log(p/\text{kPa}) = 7.47799 - 3612.44/(44.906 + T)$	Antoine eq., liquid	
	25	0.086 supercooled liquid value	GC-retention data, liquid	Hinckley <i>et al.</i> 1990
	25	0.094 supercooled liquid value	GC-retention data, liquid	
		$\log(p/\text{Pa}) = 11.18 - 3642/T$	regression eq., liquid	
	~15–110	$\log(p/\text{mmHg}) = 28.549 - 12082/T$	literature data, Antoine eq.	Oja & Suuberg 1997
	~15–110	$\log(p/\text{mmHg}) = 28.388 - 12024/T$	effusion data, Antoine eq.	
	300.85 K	0.00114	Knudsen effusion technique	Oja & Suuberg 1998
	312.85 K	0.00575		
	320.75 K	0.0162		
	327.75 K	0.0355		
	333.25 K	0.0620		
	345.55 K	0.204		
	347.25 K	0.258		
	318–363 K	$\ln(p/\text{Pa}) = 33.281 - 12024/T$	Clausius-Clapeyron eq.	Oja & Suuberg 1998
Phenanthrene	recommended value at 25 °C: $p^s = 0.001 \pm 0.0002 \text{ Pa}$			
	203.6–346.8	$\log(p/\text{mmHg}) = 7.771 - 2990/T$	static isoteniscopic method	Mortimer & Murphy 1923
		$\log(p/\text{mmHg}) = 12.780 - 4740/T$ , mean exptl temp 42 °C	effusion	Inokuchi <i>et al.</i> 1952
	36.7	0.0853	effusion	Bradley & Cleasby 1953
	39.85	0.1187		
	42	0.1600		
	46.7	0.2466		
	48.8	0.2973, 0.30		
	39.15	0.1080		
	42.1	0.148		
	44.62	0.1933		
	46.7	0.2426		
	49.65	0.3213		
	37–50	$\log(p/\text{mmHg}) = 10.388 - 4519/T$	effusion	Bradley & Cleasby 1953
	0–60	$\log(p/\text{mmHg}) = 16.00 - 5008/T$ (?)	effusion	Hoyer & Peperle 1958
	176–379	$\log(p/\text{mmHg}) = 7.26082 - 2379.04/(203.76 + t)$	Antoine eq., liquid	Zwolinski & Wilhoit 1971
	118.2–340	$\log(p/\text{mmHg}) = (-0.2185 \times 14184.0/T) + 7.936781$	Antoine eq.	Weast 1972–73
	100	30.40 measured range 100–150 °C	inclined-piston manometry	Osborn & Douslin 1975
	105	41.20		
	110	54.66		
	115	73.59		
	120	95.99		
	125	124.79		
	130	161.05		
	135	207.18		
	140	264.91		
	145	335.30		
	150	420.76		
	51.6	0.465 measured range 51.6–90.3 °C	gas saturation	Macknick & Prausnitz 1979
	57	0.813		
	61.85	1.321		
	67.35	2.120		
	71.8	3.093		

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TABLE 3. Vapor pressures and reported equations for temperature dependence of aromatic hydrocarbons—Continued

Compound	$t/^\circ\text{C}, T/\text{K}$ or temp range	Vapor pressure or reported equations: ( $p^S/\text{Pa}$ )	Method	Reference
Phenanthrene (cont'd)	78.9	5.653		
	83.4	8.892		
	90.3	14.532		
	51.6–90.3	$\ln(p/\text{Torr}) = 26.648 - 10484/T$	Clapeyron eq., solid	Macknick & Prausnitz 1979
	42–62	$\log(p/\text{Pa}) = 14.144 - 4726.6/T$	torsion-effusion	de Kruif 1980
	42–62	$\log(p/\text{Pa}) = 14.146 - 4726.6/T$	weighing-effusion	
	42–62	$\log(p/\text{Pa}) = 14.529 - 5243.6/T$		
	25	0.018	extrapolation from data	de Kruif 1980
	10.4	0.002 19 for temp range 10.4–40 °C	gas saturation	Sonnefeld <i>et al.</i> 1983
	10.35	0.002 22, 0.002 11, 0.002 38		
	18.85	0.007 38, 0.007 31, 0.007 49		
	29.5	0.0262, 0.0271, 0.0268		
	38.65	0.0899, 0.0917, 0.0889		
	38.65	0.0849		
	38.8	0.0863, 0.0844, 0.0865		
	38.9	0.0902, 0.0922, 0.0906		
	25	0.0161		
	10–50	$\log(p/\text{Pa}) = 14.852 - 4962.7/T$	gas saturation	Sonnefeld <i>et al.</i> 1983
	25	0.0704 supercooled liquid value	GC retention data	Yamasaki <i>et al.</i> 1984
	230–340	$\log(p/\text{kPa}) = 6.01392 - 2039.351/(168.569 + t)$	Nelson & Senseman 1992 data	Boublik <i>et al.</i> 1984
	203.6–347	$\log(p/\text{kPa}) = 6.613 35 - 2593.134/(224.402 + t)$	Mortimer & Murphy data	Boublik <i>et al.</i> 1984
	49.75	0.340	gas saturation method	Sato <i>et al.</i> 1986
	51.45	0.420		
	55.35	0.655		
	59.85	1.05		
	62.05	1.34		
	64.65	1.73		
	66.35	2.03		
	70.05	2.98		
	72.85	3.75		
	74.65	4.42		
	50–75	$\ln(p/\text{Pa}) = 20.3950 - 3931.20/(t - 139.743)$	Antoine eq., exptl data	Sato <i>et al.</i> 1986
	296–315 K	$\log(p/\text{kPa}) = 10.305 - 4444/T$	Antoine eq., solid	Stephenson & Malanowski 1987
	313–363 K	$\log(p/\text{kPa}) = 10.701 62 - 4552.30/T$	Antoine eq., solid	
	373–423 K	$\log(p/\text{kPa}) = 6.648 12 - 2513.514/(-65.345 + T)$	Antoine eq., liquid	
	391–613 K	$\log(p/\text{kPa}) = 7.171 86 - 3235.19/(12.908 + T)$	Antoine eq., liquid	
	25	0.111, 0.069	GC retention data, liquid	Bidleman 1984
	25	0.134, 0.10	GC retention data, liquid	Hinckley <i>et al.</i> 1990
		$\log(p/\text{Pa}) = 11.46 - 3716/T$	regression eq., liquid	
	303.49 K	0.0357	Knudsen effusion method	Oja & Suuberg 1998
	310.37 K	0.0909		
	313.92 K	0.140		
	317.94 K	0.227		
	321.25 K	0.323		
	332.93 K	0.993		
	303–333 K	$\ln(p/\text{Pa}) = 34.387 - 11423/T$ recommended value at 25 °C: $p^S = 0.02 \pm 0.005 \text{ Pa}$		
Pyrene		$\log(p/\text{mmHg}) = 12.903 - 5230/T$ ; mean exptl temp 79 °C 0.1147 measured range 69.8–85 °C	effusion	Inokuchi <i>et al.</i> 1952
	68.9	0.1880	effusion	Bradley & Cleasby 1953
	74.15	0.263, 0.274		
	78.1	0.2746		
	81.7	0.3893		
	82.65	0.4093		
	85	0.1440		
	71.75	0.2226		
	75.85	0.2880		
	82.7	0.4053		
	82.25	0.5066		
	85			
	69–85	$\log(p/\text{mmHg}) = 10.270 - 4904/T$	effusion	Bradley & Cleasby 1953
	25–90	$\log(p/\text{mmHg}) = 12.00 - 5248/T$	effusion	Hoyer & Peperle 1958
	10.5	$(9.20, 9.21, 9.53) \times 10^{-5}$ for temp range 10.5–40 °C $(3.35, 3.35, 3.39) \times 10^{-4}$	gas saturation	Sonnefeld <i>et al.</i> 1983
	20.39	$(1.10, 1.09, 1.03) \times 10^{-4}$		
	30			

TABLE 3. Vapor pressures and reported equations for temperature dependence of aromatic hydrocarbons—Continued

Compound	$t/^\circ\text{C}, T/\text{K}$ or temp range	Vapor pressure or reported equations: ( $p/\text{kPa}$ )	Method	Reference
Pyrene (cont'd)	39.34	$(3.31, 3.47, 3.25) \times 10^{-3}$		
	39.45	$(3.41, 3.20) \times 10^{-3}$		
	25	$6.00 \times 10^{-4}$		
	10–50	$\log(p/\text{kPa}) = 12.748 - 4760.73/T$	gas saturation	Sonnefeld <i>et al.</i> 1983
	25	0.0113, 0.049	GC retention data, liquid	Bödeman 1984
	25	$1.64 \times 10^{-3}$ supercooled liquid value	GC retention data	Yamasaki <i>et al.</i> 1984
	200–394	$\log(p/\text{kPa}) = 4.75092 - 1127.529/(16.02 + t)$	Anoine eq.	Boublik <i>et al.</i> 1984
	200–395	$\log(p/\text{mmHg}) = 5.6184 - 1122.0/(t + 15.2)$	Anoine eq.	Dean 1985
	298–401 K	$\log(p/\text{kPa}) = 10.75452 - 5072.78/T$	Anoine eq., solid	Stephenson & Malanowski 1985
	360–419 K	$\log(p/\text{kPa}) = 11.35052 - 5286.784/T$	Anoine eq., solid	
	511–668 K	$\log(p/\text{kPa}) = 5.5106 - 1743.57/(-170.83 + T)$	Anoine eq., liquid	
	80.11	0.30 solid phase	pressure gauge	Sasse <i>et al.</i> 1988
	90.10	0.764		
	100.11	1.853		
	110.14	4.360		
	120.10	9.213, 9.40		
	129.99	19.20		
	134.18	26.80		
	139.97	37.07		
	80.1–140	$\log(p/\text{mmHg}) = 8.654859 - 2967.129/(t + 182.314)$	Anoine eq., exptl solid	
	140–194	$\log(p/\text{mmHg}) = 5.62672 - 1553.755/(t + 112.964)$	Anoine eq., exptl liquid	Sasse <i>et al.</i> 1988
	139.93	40.80 liquid phase	pressure gauge	
	144.90	53.06		
	149.62	68.66		
	159.75	112.5		
	169.61	178.8		
	179.45	279.4		
	189.25	405.7		
	194.16	490.1		
	25	0.0158, 0.0144 supercooled liquid values $\log(p/\text{kPa}) = 11.92 - 4104/T$	GC retention data regression eq., liquid	Hinckley <i>et al.</i> 1990
	230.10 K	0.00963	Knudsen effusion method	Oja & Suuberg 1998
	330.14 K	0.0243		
	341.13 K	0.0209		
	346.14 K	0.0852		
	346.14 K	0.164		
	357.14 K	0.428		
	366.17 K	0.945		
	308–398 K	$\ln(p/\text{Pa}) = 33.856 - 12400/T$ recommended value at 25 °C: $p^s = 0.0006 \pm 0.0001 \text{ Pa}$		
Fluoranthene	25–85	$\log(p/\text{mmHg}) = 12.67 - 5357/T$	effusion	Hoyer & Peperle 1958
	20	0.0007	OECD methods	Schmidt-Bleek <i>et al.</i> 1982
	10.88	$(2.17, 2.05, 2.15, 2.57) \times 10^{-4}$ for temp range 10.5–40 °C	gas saturation	Sonnefeld <i>et al.</i> 1983
	20.25	$(7.07, 7.39, 7.25, 7.63) \times 10^{-4}$		
	29.79	$(2.03, 1.99) \times 10^{-3}$		
	29.8	$(2.17, 2.20) \times 10^{-3}$		
	38.9	$(5.81, 5.67, 5.58) \times 10^{-3}$		
	38.9	$(5.77, 5.46, 5.45) \times 10^{-3}$		
	25	0.00123		
	10–50	$\log(p/\text{kPa}) = 11.901 - 4415.56/T$	gas saturation	Sonnefeld <i>et al.</i> 1983
	25	0.00124	gen. col.-RPLC	Wasik <i>et al.</i> 1983
	25	0.00695 supercooled liquid value	GC retention data	Yamasaki <i>et al.</i> 1984
	197–384	$\log(p/\text{kPa}) = 5.45017 - 1717.489/(114.025 + t)$	Anoine eq.	Boublik <i>et al.</i> 1984
	298–383 K	$\log(p/\text{kPa}) = 11.96071 - 5348.06/T$	Anoine eq., solid	Stephenson & Malanowski 1987
	503–658 K	$\log(p/\text{kPa}) = 6.67549 - 2957.01/(-24.15 + T)$	Anoine eq., liquid	
	25	0.0154, 0.0067	GC retention data, liquid	Bidleman 1984
	25	0.00861, 0.00625	GC retention data, liquid	Hinckley <i>et al.</i> 1990
		$\log(p/\text{kPa}) = 11.35 - 4040/T$	regression eq., liquid	
	recommended value at 25 °C: $p^s = 0.00123 \text{ Pa}$			
Chrysene	80–145	$\log(p/\text{mmHg}) = 13.07 - 6340/T$	effusion	Hoyer & Peperle 1958
	117–144	$\log(p/\text{kPa}) = 14.937 - 6225.5/T$	torsion-effusion	de Kruij 1980
	117–144	$\log(p/\text{kPa}) = 14.848 - 6189/T$	weighing-effusion	
	117–144	$\log(p/\text{kPa}) = 14.904 - 6210/T$		
	25	$5.70 \times 10^{-7}$	extrapolated	
	25	$2.306 \times 10^{-4}$ supercooled liquid value	GC retention data	Yamasaki <i>et al.</i> 1984
	358–463 K	$\log(p/\text{kPa}) = 11.445 - 6160/T$	Anoine eq., solid	Stephenson & Malanowski 1987
	recommended value at 25 °C: $p^s = 5.7 \times 10^{-7} \text{ Pa}$			

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TABLE 3. Vapor pressures and reported equations for temperature dependence of aromatic hydrocarbons—Continued

Compound	<i>t</i> /°C, <i>T</i> /K or temp range	Vapor pressure or reported equations: ( <i>p</i> <sup>s</sup> /Pa)	Method	Reference
Triphenylene	65–125	$\log(p/\text{mmHg}) = 12.89 - 6154/T$	effusion	Hoyer & Peperle 1958
	108–133	$\log(p/\text{Pa}) = 14.919 - 6053/T$	torsion-effusion	de Kruif 1980
	108–133	$\log(p/\text{Pa}) = 14.835 - 6016.6/T$	weighing-effusion	
	108–133	$\log(p/\text{Pa}) = 14.881 - 6037.5/T$		
	25	$2.30 \times 10^{-6}$	extrapolated	
	25	$2.266 \times 10^{-4}$ supercooled liquid value	GC retention data	Yamasaki <i>et al.</i> 1984
	363–468 K	$\log(p/\text{kPa}) = 9.435 - 5620/T$	Anotine eq., solid	Stephenson & Malanowski 1987
	600–720 K	$\log(p/\text{kPa}) = 6.8974 - 3527/T$	Anotine eq., liquid	
	recommended value at 25 °C: $p^s = 2.30 \times 10^{-6}$ Pa			
		$\log(p/\text{mmHg}) = 11.485 - 6130/T$ , mean exptl temp 186 °C	effusion	Inokuchi <i>et al.</i> 1952
Naphthalene	146–173	$\log(p/\text{Pa}) = 14.984 - 6722/T$	torsion-effusion	de Kruif 1980
	146–173	$\log(p/\text{Pa}) = 14.838 - 6659/T$	weighing-effusion	
	146–173	$\log(p/\text{Pa}) = 14.910 - 6690.3/T$	mean value	
	25	$9.30 \times 10^{-9}$	extrapolated	
	276–489 K	$\log(p/\text{kPa}) = 11.505 - 5640/T$	Anotine eq., liquid	Stephenson & Malanowski 1987
	113.4	0.003 44	Knudsen effusion method	Oja & Suuberg 1998
	129.78	0.0199		
	139.56	0.0535		
	145.44	0.0496		
	160.19	0.322		
	172.88	0.584		
	198.99	4.81		
	386–472 K	$\ln(p/\text{Pa}) = 33.594 - 15151/T$	Clausius-Clapeyron eq.	Oja & Suuberg 1998
	recommended value at 25 °C: $p^s = 9.30 \times 10^{-9}$ Pa			
Benz[ <i>a</i> ]anthracene	60–120	$\log(p/\text{mmHg}) = 13.68 - 6250/T$	effusion	Hoyer & Peperle 1958
	104–127	$\log(p/\text{mmHg}) = 11.528 - 5461/T$	effusion	Kelly & Rice 1964
	57–117	$\log(p/\text{atm}) = 10.045 - 5925/T$	Knudsen wt loss effusion	Murray <i>et al.</i> 1974
		$1.47 \times 10^{-5}$	extrapolated	Murray <i>et al.</i> 1974
	100–123	$\log(p/\text{Pa}) = 15.013 - 5943.4/T$	torsion-effusion	de Kruif 1980
		$\log(p/\text{Pa}) = 14.913 - 6907/T$	weighing-effusion	
		$\log(p/\text{Pa}) = 14.968 - 5928/T$	mean value	
	25	$7.30 \times 10^{-6}$	extrapolated	
	13.81	$(8.05, 6.06, 1.13) \times 10^{-6}$ measured range 13.81–50 °C	gas saturation	Sonnefeld <i>et al.</i> 1983
	25.1	$(2.66, 2.56, 2.81) \times 10^{-5}$		
	40.12	$(1.39, 1.41, 1.36, 1.31) \times 10^{-4}$		
	40.85	$(1.17, 1.21, 1.20) \times 10^{-4}$		
	49.56	$(3.87, 3.85, 3.88) \times 10^{-4}$		
	25	$2.80 \times 10^{-5}$		
	10–50	$\log(p/\text{Pa}) = 9.684 - 4246.51/T$	gas saturation	Sonnefeld <i>et al.</i> 1983
	25	$2.506 \times 10^{-4}$ supercooled liquid value	GC retention data	Yamasaki <i>et al.</i> 1984
330–390 K		$\log(p/\text{kPa}) = 12.0507 - 5925/T$	Anotine eq., solid	Stephenson & Malanowski 1987
	377–400 K	$\log(p/\text{kPa}) = 10.653 - 5461/T$	Anotine eq., solid	
	25	$5.43 \times 10^{-4}$ supercooled liquid value	GC retention data	Hinckley <i>et al.</i> 1990
		$\log(p/\text{Pa}) = 12.63 - 4742/T$	regression eq., liquid	
	recommended value at 25 °C: $p^s = 2.8 \times 10^{-5}$ Pa			
	85–158	$\log(p/\text{atm}) = 9.601 - 6181/T$	Knudsen wt loss effusion	Murray <i>et al.</i> 1974
	25	$7.33 \times 10^{-7}$	extrapolated	
	25	$1.204 \times 10^{-5}$ supercooled liquid value	GC retention data	Yamasaki <i>et al.</i> 1984
		$\log(p/\text{kPa}) = 11.6067 - 6181/T$	Anotine eq., solid	Stephenson & Malanowski 1987
358–431 K	25	0.001 07, 0.0003	GC retention data, liquid	Bidleman 1984
	25	$2.35 \times 10^{-5}, 7.28 \times 10^{-6}$	GC retention data, liquid	Hinckley <i>et al.</i> 1990
		$\log(p/\text{Pa}) = 11.59 - 4989/T$	regression eq., liquid	
	recommended value at 25 °C: $P^s = 7.0 \times 10^{-7}$ Pa			
	86–150	$\log(p/\text{atm}) = 9.736 - 6220/T$	Knudsen wt loss effusion	Murray <i>et al.</i> 1974
	25	$7.40 \times 10^{-7}$	extrapolated value	
	25	$1.347 \times 10^{-5}$ supercooled liquid value	GC retention data	Yamasaki <i>et al.</i> 1984
		$\log(p/\text{kPa}) = 11.7417 - 6220/T$	Anotine eq., solid	Stephenson & Malanowski 1987
	25	$2.53 \times 10^{-5}$ supercooled liquid value	GC retention data, liquid	Hinckley <i>et al.</i> 1990
	25	$1.02 \times 10^{-5}$ supercooled liquid value	GC retention data, liquid	
Benz[e]pyrene		$\log(p/\text{Pa}) = 11.11 - 4803/T$	regression eq., liquid	
	recommended value at 25 °C: $P^s = 7.4 \times 10^{-7}$ Pa			
	110–180	$\log(p/\text{mmHg}) = 13.95 - 7260/T$	effusion	Hoyer & Peperle 1958
		$\log(p/\text{mmHg}) = 14.350 - 6770/T$ ; mean exptl temp 142 °C	effusion	Inokuchi <i>et al.</i> 1952
	20	$2 \times 10^{-5}$	OECD methods	Schmidt-Bleek <i>et al.</i> 1982

TABLE 3. Vapor pressures and reported equations for temperature dependence of aromatic hydrocarbons—Continued

Compound	<i>t</i> /°C, <i>T</i> /K or temp range	Vapor pressure or reported equations:	Method	Reference
Perylene (cont'd)	383–453 K	$\log(p/\text{kPa}) = 13.075 - 7260/T$	Antoine eq., solid	Stephenson & Malanowski 1987
	383–518 K	$\log(p/\text{kPa}) = 12.9379 - 7210/T$	Antoine eq., solid	
	124.18	0.0114	Knudsen effusion method	Oja & Suuberg 1998
	373.22	0.0164		
	131.02	0.0249		
	139.96	0.0373		
	141.87	0.0638		
	393–424 K	$\ln(p/\text{Pa}) = 35.702 - 15955/T$ recommended value at 25 °C: $p^S = 7.3 \times 10^{-7}$ Pa	Clausius-Clapeyron eq.	Oja & Suuberg 1998
Benzo[ <i>k</i> ]fluoranthene	90–157	$\log(p/\text{atm}) = 10.885 - 6792/T$ (preliminary values only)	Knudsen wt loss effusion	Murray <i>et al.</i> 1974
	25	$2.08 \times 10^{-5}$ supercooled liquid value	GC retention data	Yamasaki <i>et al.</i> 1984
	363–430 K	$\log(p/\text{kPa}) = 12.8907 - 6792/T$	Antoine eq., solid	Stephenson & Malanowski 1987
9-Phenylanthracene	353–426 K	recommended value at 25 °C: $p^S = 1.3 \times 10^{-7}$ Pa	Antoine eq., solid	Stephenson & Malanowski 1987
	430–510 K	$\log(p/\text{kPa}) = 12.4633 - 6018.5/T$	Antoine eq., solid	Stephenson & Malanowski 1987
		$\log(p/\text{kPa}) = 6.7183 - 4409.9/T$	Antoine eq., solid	
		recommended value at 25 °C: $p^S = 7.3 \times 10^{-7}$ Pa		
9,10-Dimethylbenz[ <i>a</i> ]-anthracene	106–135	$\log(p/\text{mmHg}) = 15.108 - 7051/T$	effusion	Kelley & Rice 1964
		$\log(p/\text{mmHg}) = 12.232 - 5897/T$	effusion, liquid	Kelley & Rice 1964
		recommended value at 25 °C: $p^S = 3.73 \times 10^{-7}$ Pa		
7,12-Demethylbenz[ <i>a</i> ]-anthracene	379–396 K	$\log(p/\text{kPa}) = 14.233 - 7051/T$	Antoine eq., solid	Stephenson & Malanowski 1987
	379–390 K	$\log(p/\text{kPa}) = 10.70417 - 5629.911/T$	Antoine eq., solid	
	396–408 K	$\log(p/\text{kPa}) = 11.357 - 5897/T$	Antoine eq., liquid	
		recommended value at 25 °C: $p^S = 3.84 \times 10^{-8}$ Pa		
20-Methylcholanthrene	128–152	$\log(p/\text{mmHg}) = 13.168 - 6643/T$	effusion	Kelley & Rice 1964
	401–425 K	$\log(p/\text{kPa}) = 12.293 - 6643/T$	Antoine eq., solid	Stephenson & Malanowski 1987
		recommended value at 25 °C:		
Benzo[ <i>ghi</i> ]perylene	116–195	$\log(p/\text{atm}) = 9.519 - 6674/T$	Knudsen wt loss effusion	Murray <i>et al.</i> 1974
	25	$1.35 \times 10^{-8}$		
	389–468 K	$\log(p/\text{kPa}) = 11.5247 - 6674/T$	Antoine eq., solid	Stephenson & Malanowski 1987
	391–513 K	$\log(p/\text{kPa}) = 10.945 - 6580/T$	Antoine eq., solid	
		recommended value at 25 °C: $p^S = 1.35 \times 10^{-8}$ Pa		
Pentacene	222–357	$\log(p/\text{Pa}) = 15.293 - 8043/T$	torsion-effusion	de Kruif 1980
	222–257	$\log(p/\text{Pa}) = 15.394 - 8095/T$	weighing-effusion	
	222–257	$\log(p/\text{Pa}) = 15.293 - 8043/T$	mean value	
	25	$1.0 \times 10^{-13}$	extrapolated	
	444–566 K	$\log(p/\text{kPa}) = 12.725 - 8260/T$	Antoine eq., solid	Stephenson & Malanowski 1987
	171.22	0.00161	Knudsen effusion method	Oja & Suuberg 1998
	184.8	0.00413		
	185.99	0.00421		
	190.97	0.0076		
	200.29	0.0171		
	210.08	0.0257		
	212	0.0515		
	443–483 K	$\ln(p/\text{Pa}) = 35.823 - 18867/T$	Clausius-Clapeyron eq.	Oja & Suuberg 1998
		recommended value at 25 °C: $p^S = 1.0 \times 10^{-13}$ Pa		
Picene	409–527 K	$\log(p/\text{Pa}) = 12.075 - 7350/T$	Antoine eq., solid	Stephenson & Malanowski 1987
Dibenz[ <i>a,c</i> ]anthracene (1,2:3,4-DBA)	152–179	recommended value at 25 °C:		
	152–179	$\log(p/\text{Pa}) = 16.25 - 7322.2/T$	torsion-effusion	de Kruif 1980
	152–179	$\log(p/\text{Pa}) = 16.011 - 7207.3/T$	weighing-effusion	
	25	$\log(p/\text{Pa}) = 10.131 - 1205/T$	mean value	
		$1.3 \times 10^{-9}$	extrapolated	
Dibenz[ <i>a,h</i> ]anthracene (1,2:3,6-DBA)	163–189	recommended value at 25 °C: $p^S = 1.3 \times 10^{-9}$ Pa		
	163–189	$\log(p/\text{Pa}) = 16.049 - 7395.4/T$	torsion-effusion	de Kruif 1980
	163–189	$\log(p/\text{Pa}) = 15.876 - 7312/T$	weighing-effusion	
	25	$\log(p/\text{Pa}) = 15.962 - 7730/T$	mean exptl. value	
	130–240	$3.7 \times 10^{-10}$	extrapolated	
	130–240	$\log(p/\text{kPa}) = 12.515 - 7420/T$	Antoine eq., solid	Stephenson & Malanowski 1987
1,2,6,7-Dibenzo-phenanthrene	398–513 K	recommended value at 25 °C: $p^S = 3.7 \times 10^{-10}$ Pa		
		$\log(p/\text{kPa}) = 12.075 - 7150/T$	Antoine eq., solid	Stephenson & Malanowski 1987
		recommended value at 25 °C:		

TABLE 3. Vapor pressures and reported equations for temperature dependence of aromatic hydrocarbons—Continued

Compound	<i>t</i> /°C, <i>T</i> /K or temp range	Vapor pressure or reported equations: ( <i>p</i> )/Pa)	Method	Reference
Coronene	160–240	$\log(p/\text{mmHg}) = 12.62 - 7675/T$	effusion	Hoyer & Peperle 1958
	154–237	$\log(p/\text{atm}) = 9.110 - 7100/T$	Knudsen wt loss effusion	Murray <i>et al.</i> 1974
	25	$1.95 \times 10^{-10}$	extrapolated from above eq.	
	427–510 K	$\log(p/\text{kPa}) = 11.1157 - 7100/T$	Antoine eq., solid	Stephenson & Malanowski 1987
	not spec.	$\log(p/\text{kPa}) = 8.886 - 5764/T$	Antoine eq., solid	
	not spec.	$\log(p/\text{kPa}) = 8.318 - 5362/T$	Antoine eq., liquid	
	147.9	0.001 91	Knudsen effusion method	Oja & Suuberg 1998
	163.6	0.006 86		
	178.1	0.0236		
	196.92	0.0895		
	209.9	0.222		
	210	0.309		
	231.13	0.927		
	421–504 K	$\ln(p/\text{Pa}) = 31.72 - 16006/T$	Clausius-Clapeyron eq.	Oja & Suuberg 1998
	recommended value at 25 °C: $p^S = 1.95 \times 10^{-10}$ Pa			

Note: t—temperature in °C, T—temperature in K, t.p.—triple point  $10^{\wedge}(A+B)-(A+B)$  in exponential form, i.e.,  $10^{(A+B)}$  regression\*—regression eq. derived from reported data given by Wania *et al.* 1994

TABLE 4. Henry's law constants and reported equations for temperature dependence of aromatic hydrocarbons

Compound	t/ °C or temp range	Henry's law const. H/(Pa·m³/mol)	Method	Reference
Benzene	30	653	concn ratio	Saylor <i>et al.</i> 1938
	4.50	187.2	headspace GC	Brown & Wasik 1974
	6.33	209.3		
	7.06	222.9		
	8.96	246.4		
	11.75	289.9		
	12.1	295.3		
	15.1	346.8		
	17.93	391.6		
	20.06	442.4		
4.5-20.06		In(H/(Pa·m³/mol)) = -4445.57/T + 21.26071		regression done by this work
	25	562	gas stripping	Mackay <i>et al.</i> 1979
	10	262	concn ratio, UV	Green & Frank 1979
	15	332		
	20	430		
	25	552		
	30	688		
		log H/atm = 8.58 - 1852.038/T		Kavanaugh & Trussell 1980
	1.0	177.8	equil. cell, conc ratio	Leighton & Calo 1981
	1.3	173.6		
0-30	11	280.3		
	13	330		
	21	469.6		
	22	482		
	27.2	597.4		
	25	554		
		In(H/atm) = 19.02 - 3964/T		
	25	595	concn ratio	Matter-Muller <i>et al.</i> 1981
	30	693.5	vapor-liquid equilibrium	Tucker <i>et al.</i> 1981
	15	396	vapor-liquid equilibrium	Sanemasa <i>et al.</i> 1981
40-100	25	610		
	35	876.6		
	45	1267		
	5	225	vapor-liquid equilibrium	Sanemasa <i>et al.</i> 1982
	15	387		
	25	608		
	35	905		
	45	1321		
		In H/MPa = 132.977 - 9463.47/T - 1.500638 × 10⁻⁵ - 16.9273 · ln T		
	20	740	EPICS	Tsonopoulos & Wilson 1983
10-30	25	562	gas stripping	Yurteri <i>et al.</i> 1987
	10	334.4	EPICS	Warner <i>et al.</i> 1987
	15	393.1		Ashworth <i>et al.</i> 1988
	20	458		
	25	535		
	30	730		
		H/(atm·m³/mol) = exp(5.334 - 3194/T)		
	25	586	concn ratio	Keeley <i>et al.</i> 1988
	25	568	concn ratio	Anderson 1992
	29	649	EPICS	Hansen <i>et al.</i> 1993
25-50	25	569	gas stripping-GC	Li <i>et al.</i> 1993
	25	535	static headspace-GC	Robbins <i>et al.</i> 1993
	30	679		
	40	890		
	45	1236		
	50	1450		
		H/(atm·m³/mol) = exp(7.14 - 3689/T)		
	10	290	equilibrium headspace	Perlinger <i>et al.</i> 1993
	15	380		
	20	460		
rm temp	25	604		
	30	741		
	25	537	equil. headspace-SPME	Zhang & Pawliszyn 1993
	25	570	equilibrium headspace	Ettre <i>et al.</i> 1993

TABLE 4. Henry's law constants and reported equations for temperature dependence of aromatic hydrocarbons—Continued

Compound	t/ °C or temp range	Henry's law const. H/(Pa·m <sup>3</sup> /mol)	Method	Reference
Benzene (cont'd)	45	912		
	60	1220		
	70	1668		
	80	1767		
	25–80	$\log(1/K_{AW}) = -2.167\ 853\ 7 + 836.2228/T$		
	23	488	gas stripping-IR	Nielsen <i>et al.</i> 1994
	25	481	EPICS	Dewulf <i>et al.</i> 1995
	2	161.5		
	6	208.2		
	10	228.3		
	18.2	365.8		
	2–25	$\ln K_{AW} = -3640/T + 0.007\ 86 \cdot Z + 10.577$		Dewulf <i>et al.</i> 1995
	4	169	gas stripping	Alaee <i>et al.</i> 1996
	10	228		
	15	326		
	20.6	411		
	25.4	552		
	30.1	744		
	34.9	874		
	4–34.9	$\ln(H/(Pa \cdot m^3/mol)) = -4672.28/T + 21.876\ 89; \Delta H_{vol} = 32.2 \text{ kJ/mol at } 20^\circ C$		
	10	287	vapor-liquid equilibrium	Turner <i>et al.</i> 1996
	15	390		
	25	640		
	35	986		
	0–50	$K_{AW} = 0.0763 + 0.002\ 11 \cdot T + 0.000\ 162 \cdot T^2$		Turner <i>et al.</i> 1996
	25	551–580	gas stripping	Hovorka & Dohnal 1997
	15	366.4	headspace equilibrium	Peng & Wan 1997
	20	436.3		
	25	538		
	30	675		
	35	766		
	40	947		
	45	1053		
		$\log K_{AW} = 7.94 - 1397/T$		
	20	438.7	headspace equilibrium	Peng & Wan 1997
	21	466	headspace equilibrium	Peng & Wan 1998
		recommended value at 25 °C: 557 Pa·m <sup>3</sup> /mol calc'd p/c		de Wolf & Lieder 1998
Toluene	4.5	178.9	headspace-GC	Brown & Wasik 1974
	6.33	203.5		
	7.06	218.1		
	8.96	244.1		
	11.75	294.2		
	12.1	299.4		
	15.1	358.8		
	17.93	413.7		
	20.06	474.3		
	25	673	gas stripping	Mackay <i>et al.</i> 1979
	1	222	equil. cell, concn ratio	Leighton & Calo 1981
	3	236		
	12.4	373		
	12.5	361		
	17.9	459		
	19.1	525		
	22.7	565		
	23	625		
	1–23	$\ln K = 18.46 - 3751/T$		
	15	381.6	vapor-liquid equilibrium	Sanemasa <i>et al.</i> 1981
	25	628		
	35	979		
	45	1404		
	15	396	vapor-liquid equilibrium	Sanemasa <i>et al.</i> 1982
	25	664		
	35	1060		
	45	1571		
	20	634	equil. headspace-GC	Schoene & Steinhanses 1985
	36.9	670		
	41.5	680		
	46	690		

TABLE 4. Henry's law constants and reported equations for temperature dependence of aromatic hydrocarbons—Continued

Compound	t/ °C or temp range	Henry's law const. H/(Pa·m <sup>3</sup> /mol)	Method	Reference
Toluene (cont'd)	20–46	$\log K_{AW} = 6.90 - 2194/T$		
	20	594	EPICS	Yurteri 1987
	25	601	gas stripping	Warner <i>et al.</i> 1987
	10	386	EPICS	Ashworth <i>et al.</i> 1988
	15	499		
	20	562		
	25	651		
	30	819		
	10–30	$H \text{ (atm} \cdot \text{m}^3/\text{mol}) = \exp(5.133 - 3024/T)$		Ashworth <i>et al.</i> 1988
	40	933	headspace-GC	Kolb <i>et al.</i> 1992
	60	1565		
	70	1915		
	80	2312		
	40–80	$\ln 1/K_{AW} = 7.61 + 2647/RT$		Kolb <i>et al.</i> 1992
	25	679	concen ratio	Anderson 1992
	28.5	722	EPICS	Hansen <i>et al.</i> 1993
	rm temp	577.6	equil. headspace-SPME	Zhang & Pawliszyn 1993
	10	293	equil. headspace	Perlinger <i>et al.</i> 1993
	15	390		
	20	499		
	25	660		
	30	838		
	25	652	static headspace-GC	Robbins <i>et al.</i> 1993
	30	835		
	40	1086		
	45	1351		
	50	1450		
	25–50	$\ln H \text{ (Pa} \cdot \text{m}^3/\text{mol}) = -3077.08/T + 16.8354$		regression done by this work
	45	1116	equil. headspace-GC	Ettre <i>et al.</i> 1993
	60	1489		
	70	1877		
	80	2427		
	45–80	$\log(1/K_{AW}) = -2.5323790 + 928.3536/T$		Ettre <i>et al.</i> 1993
	25	631	gas stripping-GC	Li <i>et al.</i> 1993
	23	676	gas stripping-IR	Nielsen <i>et al.</i> 1994
	2	175	modified EPICS	Dewulf <i>et al.</i> 1995
	6	203		
	10	250		
	18.2	424		
	25	555		
	2–25	$\ln K_{AW} = -4064/T + 0.00834 \cdot Z + 12.40$		Turner <i>et al.</i> 1996
	11.0	375.6	vapor-liquid equilibrium	
	15	460		
	25	684		
	35	1202		
	0–50	$K_{AW} = 0.115 - 0.00474 \cdot T + 0.000465 \cdot T^2$		Turner <i>et al.</i> 1996
	15	390.5	headspace equilibrium	Peng & Wan 1997
	20	475.3		
	25	605		
	30	774		
	35	984		
	40	1104		
	45	1309		
	20	$\log K_{AW} = 7.94 - 1621/T$		Peng & Wan 1997
	21	482.6	headspace equilibrium	Peng & Wan 1998
	recommended value at 25 °C: 660 Pa·m <sup>3</sup> /mol, calc'd from p/c	489	headspace equilibrium	de Wolf & Lieder 1998
Ethylbenzene	4.5	187.5	headspace GC	Brown & Wasik 1974
	6.33	217.2		
	7.06	235.1		
	8.96	265		
	11.75	329		
	12.1	333.6		
	15.1	409.7		
	17.93	480.2		
	20.06	559.1		
	4.5–20.6	$\ln(H/(Pa \cdot m^3/mol)) = -5838.34/T + 26.27571$		regression done by this work
	25	854	gas stripping	Mackay <i>et al.</i> 1979

TABLE 4. Henry's law constants and reported equations for temperature dependence of aromatic hydrocarbons—Continued

Compound	t/ °C or temp range	Henry's law const. H/(Pa·m <sup>3</sup> /mol)	Method	Reference
Ethylbenzene (cont'd)	15	418	vapor-liquid equil.-GC	Sanemasa <i>et al.</i> 1981
	25	734.4		
	35	1211		
	45	1436		
	15	459	vapor-liquid equil.-GC	Sanemasa <i>et al.</i> 1982
	25	797		
	35	1339		
	45	2016		
	38–280	ln H/MPa = 142.152 – 10780.8/T – 16.9701 × 10 <sup>6</sup> – 18.3797 · ln T		
	25	653	gas stripping	Heidman <i>et al.</i> 1985
	10	330	EPICS	Warner <i>et al.</i> 1987
	15	457		Ashworth <i>et al.</i> 1988
	20	609		
	25	798		
	30	106		
	10–30	H/(atm·m <sup>3</sup> /mol) = exp(11.92 – 4994/T)		
	25	788	static headspace-GC	Robbins <i>et al.</i> 1993
	30	1034		
	40	1662		
	25–40	ln(H/(Pa·m <sup>3</sup> /mol)) = –4624.08/T + 22.18509		regression done by this work
	rm temp	577.6	equil. headspace-SPME	Zhang & Pawliszyn 1993
	2.0	180		Dewulf <i>et al.</i> 1993
	6.0	194		
	10.0	257		
	18.2	497		
	25	669		
	2–25	ln K <sub>AW</sub> = –4567/T + 0.01047 · Z + 14.001		
	25	756	gas stripping-GC	Li <i>et al.</i> 1993
	25	895	vapor-liquid equil.	Turner <i>et al.</i> 1996
	5–45	K <sub>AW</sub> = 0.0500 + 0.00487 · T + 0.000250 · T <sub>2</sub>		Turner <i>et al.</i> 1996
	10	306	equil. headspace	Perligner <i>et al.</i> 1993
	15	427.6		
	20	582.6		
	25	660		
	30	1044		
		recommended value at 25 °C: 843 Pa·m <sup>3</sup> /mol, calc'd from p/c		
<i>o</i> -Xylene	15	299	vapor-liquid equil.	Sanemasa <i>et al.</i> 1982
	25	526		
	35	844		
	45	1323		
	20	426	EPICS	Yurteri <i>et al.</i> 1987
	10	289	EPICS	Ashworth <i>et al.</i> 1988
	15	366		
	20	480		
	25	493		
	30	634		
	10–30	H/(atm·m <sup>3</sup> /mol) = exp(5.541 – 3220/T)		
	40	1067	headspace-GC	Kolb <i>et al.</i> 1992
	60	2114		
	70	2825		
	80	2966		
	40–80	ln 1/K <sub>AW</sub> = 7.61 + 2647/RT		
	25	592	conc ratio	Kolb <i>et al.</i> 1992
	25	506	static headspace - GC	Anderson 1992
	30	637		Robbins <i>et al.</i> 1993
	40	1104		
	45	1074		
	50	1175		
	25–50	ln(H/(Pa·m <sup>3</sup> /mol)) = 3397.97/T + 17.67818		regression of Robbin 1993
	rm temp	537	equil. headspace-SPME	Zhang & Pawliszyn 1993
	25	485	gas stripping-GC	Li <i>et al.</i> 1993
	2	133	modified EPICS	Dewulf <i>et al.</i> 1995
	6	118		
	10	155		
	18.2	325		
	25	429		

TABLE 4. Henry's law constants and reported equations for temperature dependence of aromatic hydrocarbons—Continued

Compound	t/°C or temp range	Henry's law const. H/(Pa·m³/mol)	Method	Reference
<i>o</i> -Xylene (cont'd)	2–25	$\ln K_{AW} = -4242/T + 0.011\ 15 \cdot Z + 12.40$		
	25	731	vapor-liquid equil.	Turner <i>et al.</i> 1996
	15–45	$K_{AW} = 0.0353 + 0.004\ 44 \cdot T + 0.000\ 131$		Turner <i>et al.</i> 1996
	recommended value at 25 °C: 551 Pa·m³/mol, calc'd from p/c			
<i>m</i> -Xylene	15	405	vapor-liquid equil.	Sanemasa <i>et al.</i> 1982
	25	731		
	35	1229		
	45	1872		
	10	416	EPICS	Ashworth <i>et al.</i> 1988
	15	503		
	20	606		
	25	754		
	30	899		
	10–30	$H/(atm \cdot m^3/mol) = \exp(6.280 - 3337/T)$		
	25	739	static headspace - GC	Robbins <i>et al.</i> 1993
	30	900		
	40	1489		
	45	1591		
	50	1652		
	25–50	$\ln(H/(Pa \cdot m^3/mol)) = -3337.45/T + 17.83472$		regression done by this work
	25	665	gas stripping-GC	Li <i>et al.</i> 1993
	2	209	modified EPICS	Dewulf <i>et al.</i> 1995
	6	204		
	10	264		
	18.2	472		
	25	615		
	2–25	$\ln K_{AW} = -4026/T + 0.008\ 46 \cdot Z + 12.123$		Turner <i>et al.</i> 1996
	15–45	$K_{AW} = 0.0683 + 0.002\ 92 \cdot T + 0.000\ 225 \cdot T^2$		
	recommended value at 25 °C: 730 Pa·m³/mol, calc'd from p/c			
<i>p</i> -Xylene	15	430	vapor-liquid equil.	Sanemasa <i>et al.</i> 1982
	25	762		
	35	1265		
	45	2052		
	10	426	EPICS	Ashworth <i>et al.</i> 1988
	15	489		
	20	654		
	25	754		
	30	958		
	10–30	$H/(atm \cdot m^3/mol) = \exp(6.931 - 3520/T)$		
	25	739	static headspace-GC	Robbins <i>et al.</i> 1993
	30	900	data same as <i>m</i> -xylene	
	40	1489		
	45	1591		
	50	1652		
	25–50	$\ln(H/(Pa \cdot m^3/mol)) = -3337.45/T + 17.83472$		regression done by this work
	25	696	gas stripping-GC	Li <i>et al.</i> 1993
rm temp		678.9	equil. headspace-SPME	Zhang & Pawliszyn 1993
	27	856	EPICS	Hansen <i>et al.</i> 1993
	35.8	1189		
	46	1576		
	27–46	$\ln(H/(kPa \cdot m^3/mol)) = -3072/T + 10.0$		
	2	176	modified EPICS	Dewulf <i>et al.</i> 1995
	6	158		
	10	252		
	18.2	468		
	25	575		
	2–25	$\ln K_{AW} = -4479/T + 0.011\ 96 \cdot Z + 13.597$		Dewulf <i>et al.</i> 1995
	15–45	$K_{AW} = 0.146 - 0.003\ 49 \cdot T + 0.000\ 392 \cdot T^2$		Turner <i>et al.</i> 1996
	recommended value at 25 °C: 690 Pa·m³/mol, calc'd from p/c			
1,2,3-Trimethylbenzene	15	241.2	vapor-liquid equil.	Sanemasa <i>et al.</i> 1982
	25	441		
	35	706		
	45	1058		
	recommended value at 25 °C: 343 Pa·m³/mol, calc'd from p/c			
1,2,4-Trimethylbenzene	15	377	vapor-liquid equil.	Sanemasa <i>et al.</i> 1982
	25	619		
	35	1042		
	45	1663		

TABLE 4. Henry's law constants and reported equations for temperature dependence of aromatic hydrocarbons—Continued

Compound	<i>t</i> /°C or temp range	Henry's law const. H/(Pa·m <sup>3</sup> /mol)	Method	Reference
1,2,4-Trimethylbenzene (cont'd)	20	475	EPICS	Yurteri <i>et al.</i> 1987
	27	704	EPICS	Hansen <i>et al.</i> 1993
	35	1135		
	45	1591		
	27-45	$\ln(H/(kPa \cdot m^3/mol)) = -4298/T + 14.0$ recommended value at 25 °C: 569 Pa·m <sup>3</sup> /mol, calc'd from p/c		
1,3,5-Trimethylbenzene	15	547	vapor-liquid equil.	Sanemasa <i>et al.</i> 1981
	25	929		
	35	1501		
	45	2466		
	15	511	vapor-liquid equil.	Sanemasa <i>et al.</i> 1982
	25	887		
	35	1465		
	45	2394		
	10	408	EPICS	Ashworth <i>et al.</i> 1988
	15	466		
	20	477		
	25	682		
	30	976		
	10-30	$H/(atm \cdot m^3/mol) = \exp(7.241 - 3628/T)$ recommended value at 25 °C: 781 Pa·m <sup>3</sup> /mol, calc'd from p/c		Ashworth <i>et al.</i> 1988
	25	704	gas stripping-GC	Li <i>et al.</i> 1993
<i>n</i> -Propylbenzene	15	594		
	25	1062	vapor-liquid equil.	Sanemasa <i>et al.</i> 1982
	35	1818		
	45	2754		
	10	576	EPICS	Ashworth <i>et al.</i> 1988
	15	741		
	20	893		
	25	1094		
	30	1388		
	10-30	$H/(atm \cdot m^3/mol) = \exp(7.835 - 3681/T)$ recommended value at 25 °C: 1040 Pa·m <sup>3</sup> /mol, calc'd p/c		
	25	1102	gas stripping-GC	Li <i>et al.</i> 1993
	10	441	equil. headspace	Perlinger <i>et al.</i> 1993
	15	629		
	20	848		
	25	1175		
	30	1550		
Cumene	25	909	calc'd from measured S	Glew & Robertson 1956
	25-80	$\log(p/x)/mmHg = -7763.72/T - 42.9215 \log T + 137.82435$		
	25	1126	gas stripping-GC	Li <i>et al.</i> 1993
	28	1323	EPICS	Hansen <i>et al.</i> 1993
	36	1547		
	46.1	2422		
	28-46.1	$\ln(H/(kPa \cdot m^3/mol)) = -3269/T + 11.0$ recommended value at 25 °C: 1466 Pa·m <sup>3</sup> /mol, calc'd from p/c		
<i>n</i> -Butylbenzene	10	542	equil. headspace	Perlinger <i>et al.</i> 1993
	15	828		
	20	1115		
	25	1692		
	30	2168		
	25	1502	gas stripping-GC	Li <i>et al.</i> 1993
Methyl ethylbenzene (isomer not specify)	15	426	EPICS	Ashworth <i>et al.</i> 1988
	20	510		
	25	565		
	30	780		
	10-30	$H/(atm \cdot m^3/mol) = \exp(5.557 - 3170/T)$ recommended value at 25 °C		Ashworth <i>et al.</i> 1988
Naphthalene	25	56	gas stripping	Southworth 1979
	25	48.9	gas stripping	Mackay <i>et al.</i> 1979
	25	44.46	gas stripping	Mackay & Shiu 1981
	20	36.5	EPICS	Yurteri <i>et al.</i> 1987
	25	74.38	wetted-wall column	Fendinger & Glotfelty 1990
	rm temp	46.61	equil. headspace-SPME	Zhang & Pawliszyn 1993

TABLE 4. Henry's law constants and reported equations for temperature dependence of aromatic hydrocarbons—Continued

Compound	t/°C or temp range	Henry's law const. H/(Pa·m³/mol)	Method	Reference
Naphthalene (cont'd)	3.7	9.65	gas stripping	Alaee <i>et al.</i> 1996
	9.4	15.4		
	15.3	21.4		
	15.5	23.1		
	20	33.2		
	25	42.6		
	25.4	45.2		
	30.2	58.6		
	35.5	79.1		
	3.7–35.5	$\ln(H/\text{Pa} \cdot \text{m}^3/\text{mol}) = -659.57/T + 22.73898; \Delta H_{\text{vol}} = 44.6 \text{ kJ/mol}$ at 20 °C		
	25	44.6	gas stripping	Shiu & Mackay 1997
	20	45.0	gas stripping	De Maagd <i>et al.</i> 1998
	recommended value at 25 °C: 43 Pa·m³/mol, calc'd from p/c			
1-Methylnaphthalene	25	26.3	gas stripping	Mackay & Shiu 1981
	25	62.0	wetted-wall	Fendinger & Glotfelty 1990
	25	24.3	gas stripping	Shiu & Mackay 1997
	4.1	10.11	gas stripping	Bamford <i>et al.</i> 1999
	11	17.39		
	18	29.17		
	25	47.78		
	31	71.67		
	$\ln K_{\text{AW}} = -48.4/RT + 0.130/R$			
	recommended value at 25 °C: 44.90 Pa·m³/mol, calc'd from p/c			
2-Methylnaphthalene	25	322	wetted-wall column	Fendinger & Glotfelty 1990
	26	20 265	EPICS	Hansen <i>et al.</i> 1993
	35.8	22 900		
	46	26 243		
	26–46	$\ln(H/\text{kPa} \cdot \text{m}^3/\text{mol}) = -1234/T + 7.0$		
	20	46.0	gas stripping	De Maagd <i>et al.</i> 1998
	4.1	13.04	gas stripping	Bamford <i>et al.</i> 1999
	11	21.04		
	18	33.19		
	25	51.28		
	31	73.31		
	$\ln K_{\text{AW}} = -42.4/RT + 0.110/R$			
	recommended value at 25 °C: 51 Pa·m³/mol, calc'd from p/c			
Biphenyl	25	41.34	gas stripping	Mackay <i>et al.</i> 1979
	25	30.4	gas stripping	Mackay & Shiu 1981
	25	19.6	wetted-wall column	Fendinger & Glotfelty 1990
	25	31.2	gas stripping	Shiu & Mackay 1997
	recommended value at 25 °C: 28 Pa·m³/mol, calc'd from p/c			
Acenaphthene	25	14.79	gas stripping	Mackay <i>et al.</i> 1979
	25	15.7	gas stripping	Mackay & Shiu 1981
	25	24.42	gas stripping	Warner <i>et al.</i> 1987
	25	6.45	wetted-wall column	Fendinger & Glotfelty 1990
rm temp	9.22		equil headspace-SPME	Zhang & Pawliszyn 1993
	25	16.2	gas stripping	Shiu & Mackay 1997
	4.1	3.52	gas stripping	Bamford <i>et al.</i> 1999
	11	6.29		
	18	10.93		
	25	18.53		
	31	28.57		
	$\ln K_{\text{AW}} = -51.9/RT + 0.133/R$			
	recommended value at 25 °C: 12.2 Pa·m³/mol, calc'd from p/c			
Acenaphthylene	25	11.55	gas stripping	Warner <i>et al.</i> 1987
	25	11.4	wetted-wall column	Fendinger & Glotfelty 1990
	4.1	2.38	gas stripping	Bamford <i>et al.</i> 1999
	11	4.27		
	18	7.46		
	25	12.68		
	31	19.61		
	$\ln K_{\text{AW}} = -52.2/RT + 0.131/R$			
	recommended value at 25 °C: 8.4 Pa·m³/mol, calc'd from p/c			
Fluorene	25	7.75	gas stripping	Mackay & Shiu 1981

TABLE 4. Henry's law constants and reported equations for temperature dependence of aromatic hydrocarbons—Continued

Compound	t/°C or temp range	Henry's law const. H/(Pa·m <sup>3</sup> /mol)	Method	Reference
Florene (cont'd)	25	11.85	gas stripping	Warner <i>et al.</i> 1987
	25	6.45	wetted-wall column	Fendinger & Glotfelter 1990
	25	9.75	gas stripping	Shiu & Mackay 1997
	20	6.50	gas stripping	De Maagd <i>et al.</i> 1998
	4.1	2.05	gas stripping	Bamford <i>et al.</i> 1999
	11	3.54		
	18	5.96		
	25	9.81		
	31	14.76		
	$\ln K_{AW} = -48.8/RT + 0.118/R$ recommended value at 25 °C: 7.87 Pa·m <sup>3</sup> /mol, calc'd from p/c			
Phenanthrene	25	5.55	gas stripping	Southworth 1979
	25	3.98	gas stripping	Mackay <i>et al.</i> 1979
	25	3.65	gas stripping	Mackay & Shiu 1981
	25	2.38	wetted-wall column	Fendinger & Glotfelter 1990
	rm temp	4.05	equil. headspace-SPME	Zhang & Pawliszyn 1993
	5.9	1.81	gas stripping	Alaei <i>et al.</i> 1996
	10.4	2.99		
	15	3.06		
	20.2	3.66		
	25.7	4.73		
	30.2	5.54		
	35.5	7.9		
	$\ln (H/(Pa·m^3/mol)) = -3262.94/T + 14.18099$ ; $\Delta H_{vol} = 29.3 \text{ kJ/mol}$ at 20 °C			
	25	3.61	gas stripping	Shiu & Mackay 1997
	20	2.90	gas stripping	De Maagd <i>et al.</i> 1998
	4.1	0.94	gas stripping	Bamford <i>et al.</i> 1999
	11	1.60		
	18	2.65		
	25	4.29		
	31	6.38		
	$\ln K_{AW} = -47.3/RT + 0.106/R$ recommended value at 25 °C: 3.2 Pa·m <sup>3</sup> /mol, calc'd from p/c			
Anthracene	25	6.59	gas stripping	Southworth 1979
	25	7.19	gas stripping	Mackay & Shiu 1981
	25	1.96	wetted-wall column	Fendinger & Glotfelter 1990
	21	3.30	gas stripping	Friesen <i>et al.</i> 1993
	rm temp	8.71	equil. headspace-SPME	Zhang & Pawliszyn 1993
	5.4	2.76	gas stripping	Alaei <i>et al.</i> 1996
	10.1	3.12		
	14.8	3.44		
	20.6	3.91		
	25	4.94		
	30.2	8.05		
	35.3	8.94		
	$\ln (H/(Pa·m^3/mol)) = -3523.78/T + 13.54418$ ; $\Delta H_{vol} = 26.9 \text{ kJ/mol}$ at 20 °C			
	4.1	1.25	gas stripping	Bamford <i>et al.</i> 1999
	11	2.12		
	18	3.50		
	25	5.64		
	31	8.36		
	$\ln K_{AW} = -46.8/RT + 0.106/R$ recommended value at 25 °C: 4.0 Pa·m <sup>3</sup> /mol, calc'd from p/c			
1-Methylphenanthrene	4.1	1.58	gas stripping	Bamford <i>et al.</i> 1999
	11	2.36		
	18	3.47		
	25	5.00		
	31	6.77		
	$\ln K_{AW} = -35.4/RT + 0.067/R$ recommended value at 25 °C:			
Fluoranthene	10	0.26	gas stripping-HPLC	ten Huischer <i>et al.</i> 1992
	20	0.64		
	35	1.63		
	40.1	2.38		
	45	5.84		

TABLE 4. Henry's law constants and reported equations for temperature dependence of aromatic hydrocarbons—Continued

Compound	t/°C or temp range	Henry's law const. H/(Pa·m <sup>3</sup> /mol)	Method	Reference
Floranthene (cont'd)	55	6.23		
	10–55	$\ln(H/(Pa\cdot m^3/mol)) = -6863.2/T + 22.91268; \Delta H_{vol} = 57 \text{ kJ/mol at } 20^\circ\text{C}$		
	20	1.10	gas stripping	De Maagd <i>et al.</i> 1998
	4.1	0.56	gas stripping	Bamford <i>et al.</i> 1999
	11	0.87		
	18	1.32		
	25	1.96		
	31	2.72		
		$\ln K_{AW} = -38.7/RT + 0.070/R$		Bamford <i>et al.</i> 1999
		recommended value at 25 °C: 1.0 Pa·m <sup>3</sup> /mol, calc'd from p/c		
Pyrene	25	1.89	gas stripping	Southworth 1979
	25	1.10	gas stripping	Mackay & Shiu 1981
	25	1.21	gas stripping	Shiu & Mackay 1997
	20	2.0	gas stripping	De Maagd <i>et al.</i> 1998
	20	0.92	gas stripping	De Maagd <i>et al.</i> 1998
	4.1	0.43	gas stripping	Bamford <i>et al.</i> 1999
	11	0.69		
	18	1.10		
	25	1.71		
	31	2.45		
		$\ln K_{AW} = -42.9/RT + 0.084/R$		Bamford <i>et al.</i> 1999
		recommended value at 25 °C: 0.92 Pa·m <sup>3</sup> /mol, calc'd from p/c		
Chrysene	rm temp	0.106	equil. headspace-SPME	Zhang & Pawliszyn 1993
	4.1	0.02	gas stripping	Bamford <i>et al.</i> 1999
	11	0.07		
	18	0.19		
	25	0.53		
	31	1.20		
		$\ln K_{AW} = -100.9/RT + 0.268/R$		Bamford <i>et al.</i> 1999
		recommended value at 25 °C: 0.065 Pa·m <sup>3</sup> /mol, calc'd from p/c		
Benz[a]fluorene	4.1	0.88	gas stripping	Bamford <i>et al.</i> 1999
	11	1.30		
	18	1.89		
	25	2.70		
	31	3.62		
		$\ln K_{AW} = -34.2/RT + 0.058/R$		Bamford <i>et al.</i> 1999
		recommended value at 25 °C: 0.058 Pa·m <sup>3</sup> /mol, calc'd from p/c		
Benz[a]anthracene	rm temp	0.101	equil. headspace-SPME	Zhang & Pawliszyn 1993
	4.1	0.15	gas stripping	Bamford <i>et al.</i> 1999
	11	0.31		
	18	0.63		
	25	1.22		
	31	2.11		
		$\ln K_{AW} = -66.4/RT + 0.159/R$		Bamford <i>et al.</i> 1999
		recommended value at 25 °C: 0.0465 Pa·m <sup>3</sup> /mol, calc'd from p/c		
Benzo[a]pyrene	10	0.022	gas stripping-HPLC	ten Hulscher <i>et al.</i> 1992
	20	0.034		
	35	0.074		
	40.1	0.092		
	45	0.11		
	55	0.239		
	10–55	$\ln(H/(Pa\cdot m^3/mol)) = -4722.58/T + 12.76655; \Delta H_{vol} = 39 \text{ kJ/mol at } 20^\circ\text{C}$		
		recommended value at 25 °C:		
Benzo[b]fluoranthene	10	0.025	gas stripping-HPLC	ten Hulscher <i>et al.</i> 1992
	20	0.051		
	35	0.119		
	40.1	0.208		
	45	0.37		
	55			
	10–55	$\ln(H/(Pa\cdot m^3/mol)) = -5449.82/T + 15.26835; \Delta H_{vol} = 45.3 \text{ kJ/mol at } 20^\circ\text{C}$		
		recommended value at 25 °C:		

TABLE 4. Henry's law constants and reported equations for temperature dependence of aromatic hydrocarbons—Continued

Compound	t/ °C or temp range	Henry's law const. H/(Pa·m <sup>3</sup> /mol)	Method	Reference
Benzo[ <i>k</i> ]fluoranthene	10	0.022	gas stripping-HPLC	ten Hulscher <i>et al.</i> 1992
	20	0.043		
	35	0.107		
	40.1	0.138		
	45	0.198		
	55	0.403		
	10–55	$\ln(H/(Pa\cdot m^3/mol)) = -5881.74/T + 16.80291; \Delta H_{vol} = 49 \text{ kJ/mol at } 20^\circ C$		
		recommended value at 25 °C:		
Benzo[ <i>ghi</i> ]perylene	10	0.019	gas stripping-HPLC	ten Hulscher <i>et al.</i> 1992
	20	0.027		
	35	0.052		
	40.1	0.054		
	45	0.066		
	55	0.087		
	10–55	$\ln(H/(Pa\cdot m^3/mol)) = 3186.73/T + 7.292\ 855; \Delta H_{vol} = 26.1 \text{ kJ/mol at } 20^\circ C$		
		recommended value at 25 °C:		
Indeno[1,2,3- <i>cd</i> ]pyrene	10	0.018	gas stripping-HPLC	ten Hulscher <i>et al.</i> 1992
	20	0.029		
	35	0.057		
	40.1	0.061		
	45	0.077		
	55	0.105		
	10–55	$\ln(H/(Pa\cdot m^3/mol)) = -36.3917/T + 8.864171; \Delta H_{vol} = 30.0 \text{ kJ/mol at } 20^\circ C$		
		recommended value at 25 °C:		

<sup>a</sup>Note: EPICS—equilibrium partitioning in closed system;  $\Delta_{vol}H$ —enthalpy change of volatilization; SPME—solid-phase microextraction

TABLE 5. Recommended physical-chemical properties at 25 °C and equations for temperature dependence equations between 5 and 50 °C, (temperature  $t$  in °C and  $T$  in K)

Compounds		Recommended properties at 25 °C	Recommended/selected temperature dependence equations between 5 and 50 °C, calc'd. values at 25 °C
Benzene	$p$ , Pa	12700±500	$\log(p/\text{kPa})=6.029\ 94-1211.033/(T-52.36)$
	$S$ , g/m <sup>3</sup>	1780±50	$\log x=-15.544\ 647+1442.4276/T+3.2831\times 10^{-5}\cdot T^2$
	$H$ , Pa·m <sup>3</sup> /mol	557	12672 Pa 1799 g/m <sup>3</sup>
Toluene	$p$ , Pa	3800±200	$\log(p/\text{kPa})=6.162\ 73-1391.005/(T-48.974)$
	$S$ , g/m <sup>3</sup>	530±20	$\ln x=-46.05+7268.85/T+1.411\times 10^{-4}T^2$
	$H$ , Pa·m <sup>3</sup> /mol	660	3805 Pa 556 g/m <sup>3</sup>
Ethylbenzene	$p$ , Pa	1270±50	$\log(p/\text{kPa})=6.08211\ 19-1424.255/(T-59.944)$
	$S$ , g/m <sup>3</sup>	160±20	$\ln x=-30.799+3986.26/T+7.9095\times 10^{-5}\cdot T^2$
	$H$ , Pa·m <sup>3</sup> /mol	843	1267 Pa 180
<i>o</i> -Xylene	$p$ , Pa	882±40	$\log(p/\text{kPa})=6.123\ 838-1474.679/(T-59.464)$
	$S$ , g/m <sup>3</sup>	170±10	N/A
	$H$ , Pa·m <sup>3</sup> /mol	551	882 Pa
<i>m</i> -Xylene	$p$ , Pa	1100±100	$\log(p/\text{kPa})=6.134\ 008-1462.266/(T-58.045)$
	$S$ , g/m <sup>3</sup>	160±16	N/A
	$H$ , Pa·m <sup>3</sup> /mol	730	1106 Pa
<i>p</i> -Xylene	$p$ , Pa	1170±100	$\log(p/\text{kPa})=6.115\ 35-1453.430/(T-57.843); 12-60\ ^\circ\text{C}$
	$S$ , g/m <sup>3</sup>	180±15	$\ln x=-27.937+3230.3/T+7.595\times 10^{-5}\cdot T^2$
	$H$ , Pa·m <sup>3</sup> /mol	690	1167 Pa 188.6 g/m <sup>3</sup>
1,2,3-Trimethylbenzene	$p$ , Pa	200	$\log(p/\text{kPa})=6.173\ 03-1593.958/(T-66.072)$
	$S$ , g/m <sup>3</sup>	70±7	$\ln x=-39.5173+5289.13/T+1.149\times 10^{-4}\cdot T^2$
	$H$ , Pa·m <sup>3</sup> /mol	343	202 Pa 63.5 g/m <sup>3</sup>
1,2,4-Trimethylbenzene	$p$ , Pa	270±20	$\log(p/\text{kPa})=6.168\ 66-1573.267/(T-64.386)$
	$S$ , g/m <sup>3</sup>	57±5	$\ln x=-8.760-868.70/T$
	$H$ , Pa·m <sup>3</sup> /mol	569	271 Pa 56.8 g/m <sup>3</sup>
1,3,5-Trimethylbenzene	$p$ , Pa	325±20	$\log(p/\text{kPa})=6.198\ 65-1569.622/(T-63.572)$
	$S$ , g/m <sup>3</sup>	50±5	$\ln x=-9.533\ 86-678.83/T$
	$H$ , Pa·m <sup>3</sup> /mol	781	322 Pa 49.6 g/m <sup>3</sup>
<i>n</i> -Propylbenzene	$p$ , Pa	450	$\log(p/\text{kPa})=6.076\ 25-1490.903/(T-66.05)$
	$S$ , g/m <sup>3</sup>	52±5	N/A
	$H$ , Pa·m <sup>3</sup> /mol	1041	450 Pa
Isopropylbenzene (cumene)	$p$ , Pa	610	$\log(p/\text{kPa})=6.061\ 49-1460.793/(T-65.373)$
	$S$ , g/m <sup>3</sup>	50±5	N/A
	$H$ , Pa·m <sup>3</sup> /mol	1466	611 Pa
<i>n</i> -Butylbenzene	$p$ , Pa	137	N/A
	$S$ , g/m <sup>3</sup>	13.8±1.2	$\ln x=-43.2390+5720.35/T+1.221\times 10^{-4}\cdot T^2; r^2=0.987$
	$H$ , Pa·m <sup>3</sup> /mol	1332	13.81 g/m <sup>3</sup>
Styrene	$p$ , Pa	880±40	$\log(p/\text{kPa})=7.394\ 5-2221.3/T$
	$S$ , g/m <sup>3</sup>	320±20	$\ln x=-19.471+1655.9/T+4.6224\times 10^{-5}\cdot T^2$
	$H$ , Pa·m <sup>3</sup> /mol	286	879 Pa 318 g/m <sup>3</sup>
Naphthalene	$p$ , Pa	10.4±1.0	$\log(p/\text{Pa})=13.59-3742/T$
	$S$ , g/m <sup>3</sup>	31.5±2.0	$\ln x=-1.541\ 17-3193.9/T$
	$H$ , Pa·m <sup>3</sup> /mol	43	10.9 Pa 33.9 g/m <sup>3</sup>
1-Methylnaphthalene	$p$ , Pa	8.84±0.4	$\log(p/\text{kPa})=6.396\ 09-2006.662/(T-60.525)$
	$S$ , g/m <sup>3</sup>	28.0±2.0	8.94 Pa
	$H$ , Pa·m <sup>3</sup> /mol	45	N/A
2-Ethynaphthalene	$p$ , Pa	4.0±0.3	$\ln(p/\text{kPa})=7.46683-3232.791/T$
	$S$ , g/m <sup>3</sup>		N/A
	$H$ , Pa·m <sup>3</sup> /mol		4.21 Pa
Biphenyl	$p$ , Pa	1.30±0.2	$\log(p/\text{kPa})=14.840-4407.1/T$
	$S$ , g/m <sup>3</sup>	7.2±0.5	$\ln x=-1.579\ 2-3669.26/T$
	$H$ , Pa·m <sup>3</sup> /mol	28.0	1.19 Pa 7.98 g/m <sup>3</sup>
Acenaphthene	$p$ , Pa	0.30±0.03	$\log(p/\text{kPa})=10.883-4290.5/T$
	$S$ , g/m <sup>3</sup>	3.80±0.20	$\ln x=-3.515\ 93-3297.48/T$
	$H$ , Pa·m <sup>3</sup> /mol	12.17	0.311 Pa 4.01 g/m <sup>3</sup>
Fluorene	$p$ , Pa	0.09±0.01	$\log(p/\text{kPa})=14.385-4616.07/T$
	$S$ , g/m <sup>3</sup>	1.90±0.10	$\ln x=0.828\ 61-4824/T$
	$H$ , Pa·m <sup>3</sup> /mol	7.87	0.08 Pa 1.98 g/m <sup>3</sup>
Anthracene	$p$ , Pa	0.001±0.0002	$\log(p/\text{Pa})=12.977-4791.89/T$
	$S$ , g/m <sup>3</sup>	0.045±0.005	$\ln x=-1.436\ 11-5307.55/T$
	$H$ , Pa·m <sup>3</sup> /mol	0.075±0.007*	0.000 804 Pa 0.044 g/m <sup>3</sup> 0.0804 g/m <sup>3</sup>
2-Methylnaphthalene	$p$ , Pa	3.96	N/A
	$S$ , g/m <sup>3</sup>	0.30	$\ln x=-1.841\ 995-4646.86/T$
			0.288 g/m <sup>3</sup>

TABLE 5. Recommended physical-chemical properties at 25 °C and equations for temperature dependence equations between 5 and 50 °C, (temperature t in °C and T in K)—Continued

Compounds	Recommended properties at 25 °C		Recommended/selected temperature dependence equations between 5 and 50 °C, calc'd. values at 25 °C	
2-Methylanthracene (cont'd)	<i>H</i> , Pa·m <sup>3</sup> /mol			
Phenanthrene	<i>p</i> , Pa	0.020±0.005	$\log(p/\text{Pa}) = 14.852 - 4962.77/T$	0.0161 Pa
	<i>S</i> , g/m <sup>3</sup>	1.10±0.20	$\ln x = -2.546\ 051 - 4053/T$	0.97 g/m <sup>3</sup>
	<i>H</i> , Pa·m <sup>3</sup> /mol	3.24		
Pyrene	<i>p</i> , Pa	0.0006±0.0001	$\log(p/\text{Pa}) = 12.748 - 4760.73/T$	0.000 603
	<i>S</i> , g/m <sup>3</sup>	0.132±0.02	$\ln x = -4.007\ 476 - 4252.03/T$	0.131 g/m <sup>3</sup>
	<i>H</i> , Pa·m <sup>3</sup> /mol	0.92		
Fluoranthene	<i>p</i> , Pa	0.00123	$\log(p/\text{Pa}) = 11.901 - 4415.56/T$	0.001 23 Pa
	<i>S</i> , g/m <sup>3</sup>	0.260±0.06	$\ln x = -1.796\ 327 - 4772.17/T$	0.209 g/m <sup>3</sup>
	<i>H</i> , Pa·m <sup>3</sup> /mol	0.96		
Chrysene	<i>p</i> , Pa	5.70×10 <sup>-7</sup>	$\log(p/\text{Pa}) = 14.848 - 6189/T$	1.23×10 <sup>-6</sup> Pa
	<i>S</i> , g/m <sup>3</sup>	0.0020	$\ln x = -7.944\ 71 - 4396.26/T$	0.0018 g/m <sup>3</sup>
	<i>H</i> , Pa·m <sup>3</sup> /mol	0.065		
Benzo[ <i>a</i> ]anthracene	<i>p</i> , Pa	2.80×10 <sup>-5</sup>	$\log(p/\text{Pa}) = 9.683 - 4246.51/T$	2.76×10 <sup>-5</sup> Pa
	<i>S</i> , g/m <sup>3</sup>	0.011±0.002	$\ln x = -3.060\ 466 - 5354.51/T$	0.0094 g/m <sup>3</sup>
	<i>H</i> , Pa·m <sup>3</sup> /mol	0.580		
Benzo[ <i>a</i> ]pyrene	<i>p</i> , Pa	7.0×10 <sup>-7</sup>	$\log(p/\text{kPa}) = 11.606\ 7 - 6181/T$	7.5×10 <sup>-7</sup> Pa
	<i>S</i> , g/m <sup>3</sup>	0.003±0.002	$\ln x = -2.596\ 38 - 6046.87/T$	0.001 63 g/m <sup>3</sup>
	<i>H</i> , Pa·m <sup>3</sup> /mol	0.0465		
Benzo[ <i>e</i> ]pyrene	<i>p</i> , Pa	7.40×10 <sup>-7</sup>	$\log(p/\text{kPa}) = 11.7417 - 6220/T$	7.58×10 <sup>-7</sup>
	<i>S</i> , g/m <sup>3</sup>	0.0050	$\ln x = -11.8754 - 2916.84/T$	0.0055 g/m <sup>3</sup>
	<i>H</i> , Pa·m <sup>3</sup> /mol	0.0467		

Note: N/A - not available or not recommended for temperature range between 5 and 50 °C.

Equations relating vapor pressure to temperature are usually based on the two-parameter Clausius–Clapeyron equation

$$\frac{d(\ln p^s)}{dT} = \Delta_{\text{vap}}H/RT^2, \quad (12)$$

where  $p$  is vapor pressure, and  $\Delta_{\text{vap}}H$  is the enthalpy of vaporization. Again assuming  $\Delta_{\text{vap}}H$  is constant over a narrow range of temperature, this gives

$$\ln p^s = -\Delta_{\text{vap}}H/RT + C, \quad (13)$$

which can be rewritten as the Clapeyron equation

$$\log p^s = A - B/T. \quad (14)$$

This can be empirically modified by introducing additional parameters to give the three parameter Antoine equation, which is the most common vapor pressure correlation used to represent experimental data [Zwolinski and Wilhoit (1971), Boublík *et al.* (1984), Stephenson and Malanowski (1987), and other handbooks]

$$\log p^s = A - B/(t + C), \quad (15)$$

where  $A$ ,  $B$  and  $C$  are constants and  $t$  often has units of °C.

Other forms of vapor pressure equations, such as the Cox equation, have also been widely used [Chao *et al.* (1983)]. Although the enthalpy of vaporization varies with temperature, for the narrow environmental temperature range considered here, it is often assumed to be constant both for the more volatile mononuclear aromatic hydrocarbons and the less volatile polynuclear aromatic hydrocarbons.

The van't Hoff equation also has been used to describe the temperature effect on HLC over a narrow range for volatile chlorinated organic chemicals [Ashworth *et al.* (1988)] and chlorobenzenes, polychlorinated biphenyls, and polynuclear aromatic hydrocarbons [ten Hulscher *et al.* (1992); Alaee *et al.* (1996)]. HLC can be expressed as the ratio of vapor pressure to solubility, i.e.,  $p/c$  or  $p/x$  for dilute solutions. Note that since  $H$  is expressed using a volumetric concentration, it is also affected by the effect of temperature on liquid density, whereas  $k_H$  using mole fraction is unaffected by liquid density [Tucker and Christian (1979)], thus

$$\ln(k_H/\text{Pa}) = \ln[(p^s/\text{Pa})/x]; \quad (16)$$

or

$$\ln(H/\text{Pa} \cdot \text{m}^3 \cdot \text{mol}^{-1}) = \ln[(p^s/\text{Pa})/(c_w^s/\text{mol} \cdot \text{m}^{-3})]. \quad (17)$$

By substituting equations for vapor pressure and solubility, the temperature dependence equation for HLC can be obtained, as demonstrated by Glew and Robertson (1956), Tsanopoulos and Wilson (1983), Heidman *et al.* (1985), and ten Hulscher *et al.* (1992).

A desirable long-term objective is to represent the available experimental data for vapor pressure, solubility and Henry's law constant by a common equation for temperature dependence but, of course, with different parameter values for each property. Since the three properties are related, the parameters are also inherently related, and thus the param-

eters for Henry's law constant could be derived directly from the parameters for solubility and vapor pressure, and consistency would be ensured. Unfortunately, this task is beyond the scope of this study, and equations are recommended for solubility and vapor pressure which can be used to estimate  $H$  by simple substitution.

#### 4. Data Compilation and Presentation

In this paper, only experimentally measured vapor pressures, aqueous solubilities and Henry's law constants are reported. Data which are calculated or estimated from structure–property correlations are not reported. We believe that it is preferable that only measured data be used to predict and evaluate the environmental fate of organic chemicals. Because of the large quantity of reported vapor pressure data, the vapor pressure equation derived from reported experimental data is selected and quoted as reported in the original publication. Correlation equations based on/or derived from experimental data from handbooks and/or review articles are also included.

Table 1 gives the physical constants and thermodynamic properties of the aromatic compounds, the enthalpies of fusion, enthalpies of vaporization, enthalpies of sublimation at the reported temperature, and references. Tables 2, 3 and 4 give the reported aqueous solubilities, vapor pressures, and Henry's law constants at reported temperatures, and methods of measurement. Correlation equations expressing the property as a function of temperature as reported in the original reference are also included if available. Because of the large amount of vapor pressure data for the mononuclear aromatic hydrocarbons, only the experimental data at 20–25 °C and reported equations are given with the specified temperature range of the measurement. For the less studied, higher melting point polynuclear aromatic hydrocarbons, all the experimental data and empirical equations are included, even if the reported temperature ranges exceed the environmental temperature ranges of 5–50 °C. Readers should be careful when applying these correlation equations to ensure that the specified temperature range applies and that the equation applies to liquid or solid states.

Plots of logarithm of aqueous solubility (Figs. 1–21), vapor pressure (Figs. 22–30), and Henry's law constant (Figs. 31–40) are given in a set of figures.

In Tables 2, 3 and 4, values of solubility, vapor pressure and Henry's law constant are selected and recommended at 25 °C. Selection of values at other temperatures, or selection of equations covering a range of temperatures, is difficult for the following reasons: in many cases there is considerable scatter in the data, equations generally apply over different temperature ranges, and are not necessarily consistent with the selected values. To obtain data at other temperatures we recommend examination of the reported data and the reported equations with subsequent assignment of a selected value and appropriate error limits. As the quality of measured data improves, it will be possible to assign equations covering the desired range in temperature. This is presently

only possible for a few well studied chemicals such as benzene for which values and equation have been selected by the IUPAC Solubility Series [Shaw (1989a)].

Table 5 gives the selected and recommended vapor pressures and aqueous solubilities at 25 °C and, where possible, recommended temperature dependence equations between 5 and 50 °C.

Whereas every effort has been made to report all quantities and equations accurately, there remains a possibility of error during data compilation. Accordingly, it is recommended that values should be checked with the original references.

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